Prof. Dr. Mag. Christoph Dellago

Professor of Computational Physics
Faculty of Physics
University of Vienna
Boltzmanngasse 5
1090 Vienna, Austria

Tel: +43 1 4277 51260

Fax: +43 1 4277 9511
Email: Christoph.Dellago@univie.ac.at
Web: comp-phys.univie.ac.at

Personal Information

Date and place of birth: 11 April 1965, Bozen (Italy)
Married, two children

Education

1984	Matura, Realgymnasium (high-school equivalent) in Bozen, Italy
1985-1991	University of Vienna, Austria, Diploma, Physics (Honors) Diploma Thesis: "Determination of the size distribution of aerosol particles from optical data: possibilities and problems" (Advisor: Prof. H. Horvath)
1992-1996	University of Vienna, Austria, Ph. D., Physics (Honors) Thesis: "Lyapunov instability of two-dimensional many-body systems" (Advisor: Prof. H. A. Posch)

Professional Experience

1990-1993	Software Developer, SIEMENS AG, Vienna, Austria
1993-1996	Research Assistant, Institute for Experimental Physics, University of Vienna
1996-1999	Schrödinger Fellow of the Austrian Science Foundation (FWF), Department of Chemistry, University of California at Berkeley
1999-2003	Assistant Professor, Department of Chemistry, University of Rochester
2003-present	Full Professor, Faculty of Physics, University of Vienna
2007-present	Head of the Computational Physics Group, Faculty of Physics, University of Vienna
2008-2009	Vice Dean of the Faculty of Physics, University of Vienna
2009-2012	Dean of the Faculty of Physics, University of Vienna
2017-present	Director of the International Erwin Schrödinger Institute for Mathematics and Physics, University of Vienna

Prizes and Awards

1996-1998	Erwin Schrödinger-Fellow of the Austrian Science Foundation
1997	Förderpreis der Stiftung Futura zur Förderung junger Südtiroler im Ausland
2005	The Raymond and Beverly Sackler Prize in the Physical Sciences awarded by Tel Aviv University on Mai 23, 2005

2014 UNIVIE Teaching Award of the University of Vienna

Teaching

Thermodynamics and Statistical Mechanics
Thermodynamics and Statistical Mechanics for Secondary School Teachers
Mathematical Methods for Physicists
Introduction to Soft Matter Physics
Stochastic Processes
Computational Statistical Mechanics
Computational Physics
Computational Chemistry
Computational Science

Professional Activities

University

- Jury member for the UNIVIE Teaching Award of the University of Vienna 2015.
- Mentor in the MUV6 Mentoring Program for Female Postdoctoral Researchers (Postdoktorandinnen und Habilitandinnen) at the Univeristy if Vienna, 2013-2014.
- Mentor in the Mentoring Program for Women at the Faculty of Physics, 2007-2009.
- Member of the Steering Committee of the Vienna Scientific Cluster (VSC), a joint high performance computing infrastructure of the University of Vienna, the Technical University of Vienna, and the University of Applied Life Sciences Vienna, since 2009.
- Member of the Steering Committee (Lenkungskreis) for the new PhD-program at the University of Vienna, 2009-2011.
- Member of the Council of the Faculty of Physics, University of Vienna, since 2014.
- Member of the joint strategic planning committee of the University of Vienna and the Technical University of Vienna on the *Development of the Vienna Scientifc Cluster – Future of High Performance Computing in Vienna*, spring 2010.
- Member of the Steering Committee for the new Teacher Training Program (Steuerungsgruppe Lehramt) of the University of Vienna, 2011-2012.
- Member of the Committee on Supercomputing of the Conference of Austrian Universities (Österreichische Universitätenkonferenz), 2011-2012.
- PhD-Defence opponent: University of Amsterdam (Netherlands), Ecole Superieure de Physique et de Chimie Industrielles Paris (France), Technical University of Leiden (Netherlands), ETH Zürich (Switzerland), EPF Lausanne (Switzerland).

Networks

- Austrian member in the Steering Committee of the ESF-Program *SimBioMa-Molecular Simulations in Biosystems and Materials Scienc*e , 2005-2011.
- Member of the Management Committee of the COST-Action MolSimu, European Union, 2007-2010.

- Austrian member in the Steering Committee of the ESF-Program *Exploring the Physics of Small Devices (EPSD***)**, 2009-2014.
- Member of the Board of the Special Focus Areas Vienna Computational Materials Laboratory (SFB ViCoM) funded by the Austrian Science Foundation, June 2010-present.

Scientific Organisations

- President of the Council of CECAM - Centre Europeenne pur le Calcul Atomique et Moleculaire, April 2014-March 2016.
- Chair of the Search Committee for the new Director of CECAM to take office January 1, 2017.
- Deputy Director of the Erwin Schrödinger Institute for Mathematical Physics (ESI), Vienna, since April 2014.
- Vice-President of the Council of CECAM - Centre Europeenne pur le Calcul Atomique et Moleculaire, April 2012-March 2014.
- Member of the Governing Board of the International Erwin Schrödinger Institute for Mathematical Physics (ESI), Vienna, since 2009.
- Representative of the member-organization CMS (Center for Computational Materials Science – University of Vienna and Technical University of Vienna) in the Council of CECAM – Centre Europeenne pur le Calcul Atomique et Moleculaire, since November 2010.
- Member of the selection committee of the "Hans and Walter Thirring Prize" of the Austrian Academy of Science (ÖAW), 2018-2022.

Scientific Societies

- President of the Chemical-Physical Society of Vienna (founded in 1869 by 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval and J. Stefan), December 2013-December 2014.
- Co-opted member of the Liquids Board of the European Physical Society, 2007-2008.
- Regular member of the Liquids Board of the European Physical Society, 2008-present.
- Chair of the Liquids Board of the European Physical Society, 2008-2011.
- Member of the Board of the Condensed Matter Division of the European Physical Society, 2008-2011.
- Member of the Board of the Austrian Society of Friends of Tel Aviv Univesity, since 2008.
- Member of the Governing Board of the Austrian Physical Society, since fall 2010.

Advisory Boards and Evaluations

- Evaluator of the Transregional Collaborative Research Centre SFB TR 6 "Physics of Colloidal Dispersions in External Fields", March 2009.
- Representative of the University of Vienna in the Advisory Board of the Vienna Science and Technology Fund (WWTF), since October 2011.
- Member of the Scientific Steering Committee (SSC) of PRACE (Partnership for Advanced Computing in Europe), since January 2012.
- Member of the Board of the University Infrastructure Program (Universitätsinfra-strukturprogramm) of the City of Vienna, since November 2012.
- Member of the panel for the Berni J. Alder CECAM Prize 2013.

- Chairman of the Jury of the Liquid Matter Prize 2014 of the European Physical Society.
- Member of the Panel „Innovative Vienna 2020“ set up to develop a policy for research, technology and innovation fort her period 2015-2020, Vienna, Fall 2014.
- Member of the International Advisory Board of the Middle European Cooperation in Statistical Physics (MECO), since February 2016.
- Member of the Advisory Board of the Scientific Advisory Board of the Doctoral Programme "Computational Interdisciplinary Modelling", University of Innsbruck, since December 2016.

Workshops and Conferences

- Organizer of the CECAM Workshop "Characterizing and Studying Transition Mechanisms and States in High Dimensional Systems", May 4-6, 2000, Lyon, France.
- Organizer of the CECAM Workshop “Finding transition pathways in complex systems”, September 28-30, 2003, Vitry-sur-Seine, France.
- Organizer of the Workshop “Stochastic and Deterministic Dynamics in Equilibrium and Nonequilibrium Systems” (together with H.A. Posch), August 25-28, 2004, Vienna, Austria.
- Organizer of the CECAM Workshop “Conformational dynamics in complex systems” (together with E. Vande-Eijnden and P. Bolhuis), June 6-17, 2005, Lyon, France.
- Organizer of the Workshop "Nonlinear dynamics meets stochastic dynamics", International Erwin Schrödinger Institute for Mathematical Physics (ESI), Vienna, April 18-20, 2007.
- Organizer of the Program "Metastability and Rare Events in Complex Systems", International Erwin Schrödinger Institute for Mathematical Physics (ESI), Vienna, February 1-April 30, 2008.
- Member of the Austrian advisory board of the 33rd Conference of the Middle European Cooperation in Statistical Physics-MECO33, Puchberg/Wels, Austria, April 14-16, 2008.
- Member of the Program Committee of “The 23rd General Conference on the Condensed Matter Division of the European Physical Society”, Warsaw, Poland, August 30-September 3, 2010.
- Organizer (together with Fabrizio Cleri and Rafal Kozubski) of the symposium “Computer modelling in nanoscience and nanotechnology: an atomic-scale perspective“ at the Fall Meeting of the EMRS 2010, Warsaw.
- Member of the Scientific Committee of the Conference “M3-Multiscale Molecular Modelling: Molecular Dynamics Computational Statistical Mechanics and Molecular Simulation Algorithms”, June 30-July 3, 2010, Edinburgh.
- Member of the Scientific Committee of the International Symposium in Commemoration of Erwin Schrödinger's Death, Erwin Schrödinger Institute for Mathematical Physics, Vienna, Austria, January 2011.
- Member of the Scientifc Committee of the main conference “Molecular Simulations in Biosystems and Material Science” of the ESF-network SimBioMa, Konstanz, Germany, April 4-8, 2011.
- Organizer of the “8th Liquid Matter Conference” (together with Prof G. Kahl, TU Vienna), September 6-10, Vienna, Austria, 2011.
- Member of the Scientific Advisory Board of the Vienna Seminar of Nobel Laureates 2011, Vienna, October 18-19, 2011.

- Member of the Program Committee of the 2012 Joint European Condensed Matter Conferences (CMD-24, CMMP-12, ECOSS-29, ECSCD-11), Edinburgh, UK, 3-7 September, 2012.
- Member of the Local Organizing Committee of ECCOMAS 2012, *European Congress on Computational Methods in Applied Sciences and Engineering*, September 10-14, 2012, Vienna, Austria.
- Organizer (together with Ivan Coluzza, Francesco Sciortino and Jure Dobnikar) of the CECAM/DaCaM workshop „Design of self-assembling materials“, Vienna, September 4-7, 2012.
- Organizer (together with Gerhard Kahl, Ernst Kozeschnik, Thomas Schrefl and Dieter Süss) of the ViCoM-CECAM-Winterschool „Phase stability and phase transitions in soft and hard materials”, St. Christoph am Arlberg, February 25-March 1, 2013.
- Member of the Program Committee of “DyProSo XXXIV – 34th International Symposium on the Dynamical Properties of Solids”, Vienna, September 15-19, 2013.
- International Coordinator of the Program “*Advanced Molecular Simulation Methods in the Physical Sciences”* , Kavli Institute for Theoretical Physics China (KITPC), Institute of Theoretical Physics(ITP), Chinese Academy of Sciences (CAS), Beijing, China, June 10-July 5, 2013.
- Member of the Scientific Advisory Board of the Workshop on “Nonequilibrium Phenomena, Spin Glasses, and Algorithms“, Beijing Satellite Meeting of STATPHYS 25, Kavli Institute for Theoretical Physics China (KITPC), July 1-5, 2013, Beijing, China.
- Member of the International Advisory Committee for the Conference in Scientific Computing (CSC 2013), Cyprus 3-6 Dec, 2013.
- International Program Committee for the 9th Liquid Matter Conference, 21-25 July 2014, Lisbon, Portugal.
- Organizer (together with Istvan Borzsak, University of West Hungary) of the “Central European Statistical Mechanics Mini-Meeting”, June 12-13, 2014, Budapest, Hungary.
- Organizer (together with Peter Bolhuis and Gerhard Hummer) of the CECAM/ESI Workshop “From trajectories to reaction coordinates: making sense of molecular simulation data“, September 16-18, 2015, Erwin Schrödinger Institute, Vienna, Austria.
- Organizer (together with Gerhard Kahl, Marcello Sega and Stefan Thurner) of MECO41 (Middle European Cooperation on Statistical Physics), February 15-17, 2016, Vienna, Austria.
- Organizer (together with Eberhard Widmann) of the Annual Meeting of the Austrian Physical Society (ÖPG-Jahretagung), September 27-29, 2016, Vienna, Austria.
- Organizer (together with Peter Bolhuis and Gerhard Hummer) of the CECAM-Lorentz Workshop “Reaction Coordinates from Molecular Trajectories”, August 19-September 2, 2016, Lorentz Center, Leiden, The Netherlands.
- Organizer (together with Gerhard Kahl) of the E-CAM Extended Software Development Workshop “Trajectory Sampling”, November 16-25, 2016, Internationale Akademie Traunkrichen, Traunkrichen, Austria.
- Organizer (together with Valentino Bianco, Ivan Coluzza, and Barbara Capone) of the CECAM/ESI Workshop “Water at interfaces: from proteins and devices“, November 29-December 2, 2016, Erwin Schrödinger Institute, Vienna, Austria.

- Organizer (together with Ivan Coluzza, Samuela Pasquali, Tamar Schlick, and Barbara Capone) of the CECAM/ESI Workshop "Challenges across Large-Scale Biomolecular and Polymer Simulations", February 21-24, 2017, Erwin Schrödinger Institute, Vienna, Austria.
- Organizer (together with P.T.Chrusciel, S. Fredenhagen, H. Grosse, A. Hoang, H. Narnhofer, W. Reiter and J. Yngvason), "Walter Thirring – In Memoriam", A symposium on the occasion of his 90th birthday, April 29, 2017, Erwin Schrödinger Institute, Vienna, Austria.
- Organizer (together with Peter Bolhuis and David Swenson) of the E-CAM Extended Software Development Workshop "Classical MD", August 14-25, 2017, Lorenzt Center, Leiden, The Netherlands.

Refereeing

Journals

Biophysical Journal, ChemPhysChem, Chemical Physics Letters, Chemical Physics, Computer Physics Communications, European Physical Journal B, Europhysics Letters, Journal of Chemical Physics, Journal of Computational Chemistry, Journal of Computational Physics, Journal of Physics A, Journal of Physical Chemistry, Journal of Physics: Condensed Matter, Journal of Statistical Mechanics, Journal of Chemical Theory and Computation, Langmuir, Molecular Physics, Nature Materials, Nature Chemistry, Nature Physics, Nature Communications, Physical Chemistry Chemical Physics, Physical Review B, Physical Review E, Physical Review Letters, PhysChemComm, Physica D, Proceedings of the National Academy of Sciences of the USA, Scientific Reports, Scripta Materialia, Journal of the American Chemical Society, Solid State Sciences, Soft Matter.

Funding Agencies

National Science Foundation (NSF, USA), Petroleum Research Fund of the American Chemical Society (PRF), The Italian National Institute for the Physics of Matter (INFM), Netherlands Organisation for Scientific Research (NWO), Israel Science Foundation (ISF), SLAC Linac Coherent Light Source (Stanford LCLS), European Research Council (ERC), Deutsche Forschungsgemeinschaft (DFG), Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften, Belgian Research Foundation–Flanders (FWO), Österreichischer Akademischer Austauschdienst (ÖAD), Schweizer Nationalfonds (SNF), Research Council of Norway, National Council for Science and Technology of Greece (ESET).

Hiring, Promotions, Fellowships

Alexander von Humboldt Foundation (Germany), University of Mainz (Germany), New York University (USA), University of Freiburg (Germany), University of Texas at Austin (USA), Haverford College (USA), University of Leuven (Belgium), Trinity College Cambridge (UK), University of Toronto (Canada), Institute of Science and Technology Austria ISTA (Austria), Ecole Normale Superieure Paris (France), Alfried Krupp von Bohlen und Halbach-Stiftung (Germany), Tiburtius Award (Berlin, Germany), Université Pierre et Marie Curie Paris (France), Italian Institute of Technology Genova (Italy), National Techanical University of Norway Trondheim (Norway).

Dissertations

University of Amsterdam (Netherlands), Ecole Superieure de Physique et de Chimie Industrielles Paris (France), Technical University of Vienna (Austria), ETH Zürich (Switzerland), EPF Lausanne (Switzerland), Univesity of Arizona (USA), University of California at Berkeley (USA), Technical University of Delft (Netherlands), University of Mainz (Germany), University of Düsseldorf (Germany), RMIT University (Australia), Technical University of Vienna (Austria), Univeristy of Innsbruck (Austria), University of Rome "La Sapienza" (Italy), University of Music and Performing Arts (Vienna, Austria), Free University of Berlin (Germany).

Research Interests

- Computer simulation methods for rare events
- Structure and dynamics of soft matter systems
- Phase transitions in nanoparticles
- Chemical reaction dynamics
- Nonequilibrium statistical mechanics
- Chaos in many-particle systems
- Confined liquids
- Structure and dynamics of water and ice
- Nucleation phenomena
- Proton transfer in aqueous media
- Machine learning approaches in physics and chemistry

Funding

Project title	Amount of Funding*	Funding Agency	Funding period
Studying Protein Folding with Parallel Transition Path Sampling	25.000,00 USD	ACS-PRF	2001-2002
Simulation of proton transport	185.997,00 EUR	FWF	2004-2008
Simulation of phase transitions in soft matter systems	270.427,50 EUR	FWF	2008-2011
Wissenschaftskolleg Computational Materials Science	396.000,00 EUR	FWF	2004-2012
SFB ViCoM – Vienna Computational Materials Laboratory; Subproject "Nucleation and self-assembly in soft matter systems: from the molecular to the mesoscopic scale" (co-PI Gerhard Kahl. TU Wien)	373.898,00 EUR	FWF	2010-2014
Initiativkolleg (IK) Computational Science-Algorithms for Graph Optimization and Their Applications in Life and Nano Sciences (co-PIs: M. Henzinger, O. Scherzer, I. Hofacker, A. von Haeseler, Uni Wien)	135.000,00 EUR (1.5 PhD-students for 3 years)	Univ. Vienna	2011-2014
Nucleation and growth in small systems	346.891,00 EUR	FWF	2012-2015

WTZ (Wissenschaftlich technische Zusammenarbeitit-scientific technical cooperation) Austria-Hungary, co-PI Prof. Istvan Borzak (University of Western Hungary), "Ice crystal nucleation in an external electric field"	4.098,00 EUR	OEAD	2012-2014
Parallel Software Suite for neural network potentials for materials simulations	107.700,00 EUR (1 PhD-student for 3 years)	VSC-School	2014-2017
Pressure amorphization of ice (uni:docs fellowship Clemens Moritz)	107.700,00 EUR (1 PhD-student for 3 years)	Univ. of Vienna	
SFB ViCoM – Vienna Computational Materials Laboratory; Subproject "Multiscale simulations of nucleation in liquid and solid solutions" (co-PI: Ernst Kozeschnik, TU Wien)	413.280,00 EUR	FWF	2014-2018
E-CAM, An e-infrastructure for software, training and consultancy in simulation and modelling, Work Package Classical MD (co-PI: Gerhard Kahl, TU Wien	176.000,00 EUR	EU	2015-2020
Marie Curie Individual Fellowship Gyorgy Hantal	166.156,80 EUR	EU	2016-2018
Non-equilibrium Fluctuations of Vacuum Trapped Nanoparticles in Single- and Double-Well Potentials (DACH-Projekt with L. Novotny, ETH Zürich)	187.341,00 EUR	FWF	2017-2021

*) In the case of group projects, the amount of funding refers to portion of funds that that went to the group of C. Dellago.

Students and Postdocs mentored

Postdocs

Mor Naor (2000-2001)
Andreas Tröster (2003-2009)
Elisabeth Schöll-Paschinger (2004-2007)
Bianca Mladek (2007-2008)
Ernesto Borrero (2009-2011)
Swetlana Jungblut (2008-2017)
Ivan Coluzza (2010-2017)
Panagiotis Theodorakis (2010-2012)
Ulf R. Pedersen (2011-2014)
Michael Grünwald (2012-2014)
Marcello Sega (2015-present)
Tobias Morawietz (2015-2016)

PhD-Students

Yanting Wang	Molecular dynamics simulation of gold nanomaterials	PhD 2004
Harald Oberhofer	Rare events in non-equilibrium processes and chemical reactions	PhD 2008
Wolfgang Lechner	Nucleation and defects interactions in colloidal suspensions	PhD 2009
Jürgen Köfinger	Water in nanopores	PhD 2009
Michael Grünwald	Transition path sampling simulations of structural phase transformations in nanocrystals under pressure	PhD 2009
Philipp Geiger	Neural networks for structure recognition: application to phase transitions in water and ice	PhD 2013
Jaffar Hasnain	Two-dimensional colloidal suspensions on regular and quasicrystalline light substrates	PhD 2015
Christian Leitold	Finding reaction coordinates in complex systems: unleashing the power of machine learning algorithms	PhD 2016
Georg Menzl	Cavitation in water at negative pressure	PhD 2017
Helmut Kühnelt	Lattice-Boltzmann simulations or air flow in flutes and organ pipes	PhD 2017
Andreas Singraber	Transition path sampling of phase transitions in nanoparticles	*current*
Carina Karner	Pathways to freezing in systems of convex polyhedra	*current*
Egon Tschurtschenthaler	Controlling nucleation rates with impurities	*current*
Clemens Moritz	Pressure induced amorphization of ice	*current*
Peter Wirnsberger	Sonocrystallization	*current*
Max Innerbichler	Non-equilibrium statistical physics of trapped nano-particles	*current*

Diploma and master students

Harald Obehofer	Calculating equilibrium free energies with nonequilibrium path sampling methods	2004
Walter Weissensteiner	Proton and hydroxide transport through water-filled pores	2004
Markus Heinz	Densities of states in systems with negative specific heat	2005
Wolfgang Lechner	Helmholtz free energies from non-equilibrium, fast switching simulations	2005

Michael Grünwald	Simulation of pressure-induced structural phase transitions in semiconductor nanocrystals	2005
Philipp Geiger	Optimal protocol for fast switching non-equilibrium processes	2008
Bernhard Reischl	Rare electric field fluctuations in liquid water	2008
Georg Menzl	Collective behavior of water in carbon nanotube membranes	2009
Jaffar Hasnain	Enhanced window sampling using CUDA enabled devices	2010
Markus Weinwurm	Spectroscopy of nanopore water	2010
Christian Leitold	Coil-to crystal transition in a polymer with short-range attractions	2011
Carina Karner	Lattice Boltzmann simulation of nucleation in binary fluids	2011
Philipp Gödl	Transition path sampling of the condensation of supersaturated water vapor	*current*
Raimund Hirmer	Condensation and freezing of nanoscopic water droplets	2013
Clemens Moritz	Geoemtrical transitions in the Ising model with periodic boundary conditions	2014
Peter Wirnsberger	A simulation study on the thermo-polarisation effect in water	2014
Mathias Höld	Thermal flow of a laser trapped nanoparticle	2017
Max Innerbichler	Stochastic time evolution of cavitation bubbles: computing free energies and diffusion constants with Bayesian statistics	2017
Michael Legenstein	Freezing of water in carbon nanotubes	*current*
Oliver Wohlfart	A neural network potential for the water-vapor interface	*current*
Alexander Hummelbrunner	Active particles at low friction in 3 dimensions	*current*
Igor Kraut	Using Steinhardt bond order parameters as features in neural netwoks for potential energy surfaces	*current*
Jakob Michl	Simulation of nucleation of carbon dioxide clathrates	*current*
Alexander Heinz	Calculation of the pH of neural network water	*current*
Victor Wenin	Kramers turnover for a particle in a bistable laser trap	*current*
Nils Clees	Liquid-ice Ih coexistence in neural network water	*current*

Matthias Kiss	A neural network potential for CO_2	*current*

Long-term visiting students

Andrew Ballard, Univesity of Maryland (2009-2010)
Clarion Tung, University of Calfornia at Berkeley (2009-2011)
Michael Adamer, University of Oxford (2013)
Tobias Morawietz, University of Bochum (2013)
Luca Ornigotti, University of Pavia (2015)
Aviel Chaimovich, MPI for Polymer Science (2016)

Publications

h-index (7.4.2016): 35
total number of citations (7.4.2016): 6061

1. H. Horvath, J. Gorraiz, W. Henrich, and C. Dellago, "A surface with variable reflectivity", *Review of Scientific Instruments* **61**, 1993 (1990).
2. H. Horvath and C. Dellago, "Optically determined properties of the aerosol during fog formation and dissipation", in *Aerosols; Science, health and environment. Proceedings of the 3rd International Aerosol Conference, 24-17 September 1990, Kyoto, Japan,* edited by S. Masuda and K. Takahashi. Pergamon Press, Oxford, 277 (1990).
3. C. Dellago and H. Horvath, "On the accuracy of the size distribution information obtained from light extinction and scattering measurements-I. Basic considerations and models", *Journal of Aerosol Science* **24**, 129 (1993).
4. H. Horvath and C. Dellago, "On the accuracy of the size distribution information obtained from light extinction and scattering measurements-II. Case studies", *Journal of Aerosol Science* **24**, 143 (1993).
5. C. Dellago and H. A. Posch, "Lyapunov exponents of systems with elastic hard collisions", *Physical Review E* **52**(3), 2401 (1995).
6. C. Dellago, L. Glatz, and H. A. Posch, "Lyapunov spectrum of the driven Lorentz gas", *Physical Review E* **52**, 4817 (1995).
7. C. Dellago, H. A. Posch and W. G. Hoover, "Lyapunov instability in a system of hard disks in equilibrium and nonequilibrium steady states", *Physical Review E* **53**, 1485 (1996).
8. H. A. Posch, C. Dellago, W. G. Hoover, and O. Kum, "Microscopic Time-Reversibility and Macroscopic Irreversibility - Still a Paradox?" in *Modern Atomistic and Organic Structural Chemistry: Josef Loschmidt's Pioneering Contributions and their Sequel*, edited by T. Schönfeld and W. Fleischhacker, Plenum, New York (1996).
9. C. Dellago and H. A. Posch, "Lyapunov instability, local curvature and the liquid-solid transition in two dimensional particle systems", *Physica A* **230**, 364 (1996).
10. C. Dellago and H. A. Posch, "Lyapunov instability in the extended XY-model: Equilibrium and nonequilibrium molecular dynamic simulation", *Physica A* **237**, 95 (1997).
11. W. G. Hoover, H. A. Posch, C. Dellago, O. Kum, C. G. Hoover, A. J. De Groot, and B. L. Holian, "Thermomechanical Particle Simulation", in *Proceedings of the International*

Conference on Nonlinear Dynamics, Chaotic and Complex Systems, 7-12 November 1995, Zakopane, Cambridge University Press (1996).

12. H. van Beijeren, J. R. Dorfman, E. G. D. Cohen, H. A. Posch, and C. Dellago, "Lyapunov Exponents from Kinetic Theory for a Dilute, Field-driven Lorentz Gas", *Physical Review Letters* **77**, 10 (1996).
13. C. Dellago and H. A. Posch, "Lyapunov instability of the boundary driven Chernov-Lebowitz model for stationary shear flow", *Journal of Statistical Physics*, **88**, 825 (1997).
14. C. Dellago and H. A. Posch, "Kolmogorov-Sinai entropy and Lyapunov spectra of a hard sphere gas", *Physica A* **240**, 68 (1997).
15. C. Dellago and H. A. Posch, "Mixing, Lyapunov instability, and the approach to equilibrium in a hard-sphere gas", *Physical Review E* **55**, R9 (1997).
16. C. Dellago and H. A. Posch, "Lyapunov spectrum and the conjugate pairing rule for a thermostatted random Lorentz gas: Numerical simulations", *Physical Review Letters* **78**, 211 (1997).
17. H. van Beijeren, J. R. Dorfman, H. A. Posch, and C. Dellago, "The Kolmogorov-Sinai Entropy for Dilute Gases in Equilibrium", *Physical Review E* **56**, 5272 (1997).
18. C. Dellago, W. G. Hoover, and H. A. Posch, "Isomorphic multifractal shear flows for hard disks via adiabatic and isokinetic nonequilibrium molecular dynamics", *Physical Review E* **57**, 4969 (1998).
19. C. Dellago, P. G. Bolhuis, F. S. Csajka, and D. Chandler, "Transition Path Sampling and the Calculation of Rate Constants", *Journal of Chemical Physics* **108**, 1964 (1998).
20. R. van Zon, H. van Beijeren, and C. Dellago, "Largest Lyapunov Exponent for Many Particle Systems at Low Densities", *Physical Review Letters* **80**, 2035 (1998).
21. C. Dellago and H. A. Posch, "Field and density dependence of the Lyapunov spectrum of the random driven Lorentz gas", *Physica D* **112**, 241 (1998).
22. C. Dellago, P. G. Bolhuis, and D. Chandler, "Efficient transition path sampling: Applications to Lennard-Jones cluster rearrangements", *Journal of Chemical Physics* **108**, 9236 (1998).
23. P. G. Bolhuis, C. Dellago and D. Chandler, "Sampling ensembles of deterministic transition pathways", *Faraday Discussion* **110**, 421 (1998).
24. C. Dellago, P. G. Bolhuis and D. Chandler, "On the calculation of reaction rate constants in the transition path ensemble", *Journal of Chemical Physics* **110**, 6617 (1999).
25. P. L. Geissler, C. Dellago, and D. Chandler, "Chemical dynamics of the protonated water cluster", *Physical Chemistry Chemical Physics* **1**, 1317 (1999).
26. P. L. Geissler, C. Dellago, and D. Chandler, "Kinetic Pathways of Ion Dissociation in Water", *Journal of Physical Chemistry B* **103**, 3706 (1999).
27. A. Torcini, C. Dellago and H. A. Posch, "Comment on: Lyapunov Exponent of a Many Body System and Its Transport Coefficients", *Physical Review Letters* **83**, 2676 (1999).
28. C. Dellago and W. G. Hoover, "Are Local Lyapunov Exponents Continuous in Phase Space?", *Physics Letters A* **268**, 330 (2000).
29. P. L. Geissler, C. Dellago, D. Chandler, J. Hutter, and M. Parrinello, "Ab initio analysis of proton transfer dynamics in $(H_2O)_3H^+$", *Chemical Physics Letters* **321**, 225 (2000).

30. P. G. Bolhuis, C. Dellago and D. Chandler, “Reaction coordinates of biomolecular isomerization”, *Proceedings of the National Academy of Sciences of the USA* **97**, 5877 (2000).

31. P. G. Bolhuis, C. Dellago, P. L. Geissler, and D. Chandler, “Transition path sampling: throwing ropes over mountains in the dark”, *Journal of Physics: Condensed Matter* **12**, A147 (2000).

32. P. L. Geissler, T. van Voorhis, and C. Dellago, “Potential energy landscape for proton transfer in $(H_2O)_3H^+$: Comparison of density functional theory and wavefunction based methods”, *Chemical Physics Letters* **324**, 149 (2000).

33. C. Dellago and W. G. Hoover, “Finite-Precision Stationary States At, and Away from, Equilibrium”, *Physical Review E* **62**, 6275 (2000).

34. T. J. H. Vlugt, C. Dellago, and B. Smit, “Diffusion of Isobutane in Silicalite studied by Transition Path Sampling”, *Journal of Chemical Physics* **113**, 8791 (2000).

35. R. Klages and C. Dellago, “Density-dependent Diffusion in the Lorentz Gas”, *Journal of Statistical Physics* **101**, 145 (2000).

36. D. Laria, J. Rodriguez, C. Dellago, and D. Chandler, “Dynamical Aspects of Isomerization and Melting Transitions in $[H_2O]_8$”, *Journal of Physical Chemistry A* **105**, 2646 (2001).

37. P. L. Geissler, C. Dellago, D. Chandler, J. Hutter, and M. Parrinello, “Autoionization in liquid water”, *Science* **291**, 2121 (2001).

38. C. Dellago, Henk v. Beijeren, Debabrata Panja, and J. R. Dorfman, “Field dependent collision rate of the driven random Lorentz gas”, *Physical Review E* **64**, 036217 (2001).

39. W. G. Hoover, H. A. Posch, C. Forster, C. Dellago, and M. Zhou, “Lyapunov Modes of Two-Dimensional Many-Body Systems; Soft Disks, Hard Disks, and Rotors”, *Journal of Statistical Physics* **109**, 765 (2002).

40. Peter G. Bolhuis, D. Chandler, C. Dellago, Phillip L. Geissler, “Transition Path Sampling: Throwing Ropes over Mountain Passes in the Dark”, *Annual Review in Physical Chemistry* **53**, 291 (2002).

41. C. Dellago, Peter G. Bolhuis, Phillip L. Geissler, “Transition Path Sampling”, *Advances in Chemical Physics* **123**, 1 (2002).

42. C. Dellago, W. G. Hoover, and H. A. Posch, “Fluctuations, Convergence Times, Correlation Functions, and Power Laws from Many-Body Lyapunov Spectra for Soft and Hard Disks and Spheres”, *Physical Review E* **65**, 056216 (2002).

43. C. Dellago, P. L. Geissler, D. Chandler, J. Hutter, M. Parrinello, “Comment on *Dissociation of Water under Pressure”, Physical Review Letters* **89**, 199601 (2002).

44. C. Dellago and D. Chandler, “Bridging the time scale gap with transition path sampling”, in *Molecular Simulation for the Next Decade*, ed. by P. Nielaba, M. Mareschal, and G. Ciccotti, Springer, Berlin (2002).

45. M. Naor, Keith Van Nostrand, and C. Dellago, “Car-Parrinello molecular dynamics simulation of the calcium ion in liquid water”, *Chemical Physics Letters* **369**, 159 (2003).

46. C. Dellago, M. Naor, and G. Hummer, “Proton Transport through Water-Filled Carbon Nanotubes”, *Physical Review Letters* **90**, 105902 (2003).

47. C. Dellago and S. Mukamel, “Simulation strategies and signatures of chaos in classical nonlinear response”, *Physical Review E* **67**, 035205 (2003).

48. C. Dellago and S. Mukamel, “Nonlinear Response of Classical Dynamical Systems to Short Pulses”, *Bulletin of the Korean Chemical Society* **24**, 1107 (2003).

49. C. Dellago and P. L. Geissler, “Monte Carlo sampling in path space: Calculating time correlation functions by transforming ensembles of trajectories”, Proceedings of *The Monte Carlo Method in the Physical Sciences: Celebrating the 50th anniversary of the Metropolis algorithm*, AIP Conference Proceedings, vol. 690 (2003).

50. Y. Wang and C. Dellago, “Structural and Morphological Transitions in Gold Nanorods: a Computer Simulation Study”, *Journal of Physical Chemistry B* **107**, 9214 (2003).

51. C. Dellago and S. Mukamel, “Simulation algorithms for multidimensional nonlinear response of classical many-body systems” *Journal of Chemical Physics* **119**, 9344 (2003).

52. W. Zhuang and C. Dellago, “Dissociation of hydrogen chloride and proton transfer in liquid glycerol: an *ab initio* molecular dynamics study”, *Journal of Physical Chemistry B* **108**, 19647 (2004).

53. P. L. Geissler and C. Dellago, “Equilibrium time correlation functions from irreversible transformations in trajectory space”, *Journal of Physical Chemistry* B **108**, 6667-6672 (2004).

54. Yanting Wang, S. Teitel, and Christoph Dellago, “Melting and equilibrium shape of icosahedral gold nanoparticles”, *Chemical Physics Letters* **394**, 257-261 (2004).

55. Christoph Dellago and Peter G. Bolhuis, “Activation Energies from Transition Path Sampling Simulations”, *Molecular Simulation* **30**, 795 (2004).

56. C. Dellago, "Transition Path Sampling", *Handbook of Materials Modeling,* Ed. S. Yip, Springer (2005).

57. Y. Wang, S. Teitel and C. Dellago, "Melting of icosahedral gold nanoclusters from molecular dynamics simulations", *Journal of Chemical Physics* **122**, 214722 (2005).

58. C. Dellago and M. M. Naor, "Dipole moment of water molecules in narrow pores", *Computer Physics Communications* **169**, 36 (2005).

59. H. Oberhofer, C. Dellago, and P. L. Geissler, "Biased sampling of non-equilibrium trajectories: Can fast switching simulations outperform conventional free energy calculation methods?", *Journal of Physical Chemistry* **109**, 6902 (2005).

60. A. Tröster and C. Dellago, "Wang-Landau Sampling with Self-adaptive Range", *Physical Review E* **71**, 066705 (2005).

61. A. Tröster, C. Dellago, and W. Schranz, "Free energies of the ϕ^4-model from Wang-Landau simulations", *Physical Review B* **72**, 094103 (2005).

62. Y. Wang, S. Teitel, and C. Dellago, "Surface driven bulk reorganization of gold nanorods", *NanoLetters* **5**, 2174 (2005).

63. Christoph Dellago, Peter G. Bolhuis, and Phillip L. Geissler, "Transition Path Sampling Methods", *Computer Simulations in Condensed Matter Systems: From Materials to*

Chemical Biology, Eds. M. Ferrario, G. Ciccotti, K. Binder, Vol.1, p.349-391, Springer-Verlag Berlin Heidelberg (2006).

64. W. Lechner, H. Oberhofer, C. Dellago, and P. L. Geissler, "Equilibrium free energies from fast-switching simulations with large time steps", *Journal of Chemical Physics* **124,** 044113/1-12 (2006).

65. Michael Grünwald, Eran Rabani, and Christoph Dellago, „Mechanism of the Wurtzite to Rocksalt Transformation in CdSe Nanocrystals“, *Physical Review Letters* **96**, 255701/1-4 (2006). (Also published in the *Virtual Journal of Nanoscale Science & Technology*, Vol. 14, Issue 2, July 2006).

66. E. Schöll-Paschinger und C. Dellago, “A proof of Jarzynski’s nonequilibrium work theorem for dynamical systems that conserve the canonical distribution”, *The Journal of Chemical Physics* **125**, 054105/1-5 (2006).

67. Christoph Dellago and Gerhard Hummer, "Kinetics and Mechanism of Proton Transport across Membrane Nanopores", *Physical Review Letters* **97**, 245901(4) (2006). (Also published in the *Virtual Journal of Biological Physics Research*, Vol. 12, Issue 12, Dec. 2006 and in the *Virtual Journal of Nanoscale Science & Technology*, Vol. 14, Issue 26, Dec. 2006).

68. M. Grünwald and C. Dellago, "Ideal gas pressure bath: a method for applying hydrostatic pressure in the computer simulation of nanoparticles", *Molecular Physics* **104**, 3709 (2006).

69. Christoph Dellago, “Transition Path Sampling and the Calculation of Free Energies”, Free Energy Calculations, Springer Series in Chemical Physics Vol. 86, Ch. Chipot and A. Pohorille (Eds.), Springer-Verlag Berlin Heidelberg, 249-276 (2007).

70. W. Lechner and C. Dellago, "On the efficiency of path sampling methods for the calculation of free energies from non-equilibrium simulations", *Journal of Statistical Mechanics: Theory and Experiment*, P04001 (2007).

71. Christoph Dellago and Peter G. Bolhuis, "Transition Path Sampling Simulations of Biological Systems", *Atomistic Approaches in Modern Biology - From quantum chemistry to molecular simulation, Topics in Current Chemistry* Vol. 268: 291-317, Springer (2007).

72. Yanting Wang, S. Teitel, and Christoph Dellago, "Effect of Surface Structure on Shape Transformations of Gold Nanorods", *Journal of Computational and Theoretical Nanoscience* ***4***, 282-290 (2007).

73. Harald Oberhofer, Christoph Dellago, Stefan Boresch, "Single molecule pulling with large time steps", *Physical Review E* **75***,* 061106 (2007). (Also published the *Virtual Journal of Ultrafast Science*, Vol. 6, Issue 7, July 2007 and in the *Virtual Journal of Biological Physics Research*, Vol. 13, Issue 12, June 2007).

74. A. Tröster and C. Dellago, "Coarse graining the ϕ^4 model: Landau-Ginzburg potentials from computer simulations", Ferroelectrics - Special Edition for V. Ginzburg **354**, 225-237 (2007).

75. Michael Grünwald, Christoph Dellago, Phillip L. Geissler, "An efficient transition path sampling algorithm for nanoparticles under pressure", *Journal of Chemical Physics* **127**, 154718 (2007).

76. Harald Oberhofer and Christoph Dellago, "Large timestep fast-switching simulations with non-volume preserving integrators for free energy calculations", *Israel Journal of Chemistry* 47, 215 (2007).

77. Jürgen Köfinger and Christoph Dellago, "Biasing the center of charge in molecular dynamics simulations with empirical valence bond models: free energetics of an excess proton in a water droplet", *Journal of Physical Chemistry B* **112**, 2349 (2008).

78. H. Oberhofer and C. Dellago, "Optimum bias for fast-switching free energy calculations", *Computer Physics Communications* **179**, 41-45 (2008).

79. Christoph Dellago and Harald A. Posch, "Realizing Boltzmann's dream: computer simulations in modern statistical mechanics", *ESI Lectures in Mathematics and Physics "Boltzmann's legacy"*, Eds. G. Gallavotti, W. L. Reiter and J. Yngvason, European Mathematical Society (2008).

80. Jürgen Köfinger, Gerhard Hummer, and Christoph Dellago, "Macroscopically Ordered Water in Nanopores", *Proceedings of the National Academy of the USA* **105**, 13218 (2008).

81. Markus Marksteiner, Philipp Haslinger, Hendrik Ulbricht, Michele Sclafani, Harald Oberhofer, Christoph Dellago, and Markus Arndt, "Gas-phase formation of large neutral alkaline-earth metal tryptophan complexes", *Journal of the American Society of Mass Spectroscopy* **19**, 1021 (2008).

82. Wolfgang Lechner, Elisabeth Schöll-Paschinger, and Christoph Dellago, "Displacement fields of point defects in two-dimensional colloidal crystals", *Journal of Physics: Condensed Matter* **20**, 404202 (2008).

83. Wolfgang Lechner and Christoph Dellago, "Accurate determination of crystal structures based on averaged local bond order parameters", *Journal of Chemical Physics* **129**, 114707 (2008).

84. Michael Grünwald, Christoph Dellago, Phillip L. Geissler, "Precision shooting: sampling long transition pathways", *Journal of Chemical Physics* **129**, 194101 (2008). (Also published in the *Virtual Journal of Nanoscale Science & Technology*, Vol. 18, Issue 2, Dec. 2008).

85. C. Dellago, “Metastability and Rare Events in Complex Systems”, *ESI News*, Vol. 3, Issue 2 (Autumn 2008).

86. Christoph Dellago and Peter G. Bolhuis, "Transition Path Sampling and other Advanced Simulation Techniques for Rare Events", pp. 167-233, *Advanced Computer Simulation Approaches for Soft Matter Sciences III*, Springer Series: A*dvances in Polymer Science,* Vol. 221, Eds. C. Holm and K. Kremer, Springer (2008).

87. Wolfgang Lechner and Christoph Dellago, "Point defects in two-dimensional colloidal crystals: simulation vs. elasticity theory", *Soft Matter* **5***,* 646 (2009).

88. Peter G. Bolhuis and Christoph Dellago, "Trajectory based rare event simulations", *Reviews of Computational Chemistry* 27, 111-210 (2010).

89. A. Tröster and C. Dellago, "The Fourier Monte Carlo Approach to Lattice Spin Models", *Computer Simulation Studies in Condensed Matter Physics XXI*, Eds. D. P. Landau, S. P. Lewis, and H. B. Schüttler, Springer, in print (2009).

90. Michael Grünwald and Christoph Dellago, "Nucleation and growth in structural transformations of nanocrystals", *Nano Letters* **9,** 2099-2102 (2009).

91. Christoph Dellago and Michael Grünwald, "Transition Path Sampling Studies of Solid-Solid Transformations in Nanocrystals under Pressure", pp. 61-884, *Trends in Computational Nanomechanics: Transcending Lengths and Time Scales*, Springer Series: Challenges and Advances in Computational Chemistry and Physics, Vol. 9, Ed. Traian Dumitrica (2010).

92. B. Reischl, J. Köfinger, C. Dellago, "The statistics of electric field fluctuations in liquid water", *Molecular Physics* **107**, 495-502 (2009).

93. H. Oberhofer and C. Dellago, "Efficient extraction of free energy profiles from non-equilibrium experiments", *Journal of Computational Chemistry* **30,** 1726-36 (2009).

94. J. Köfinger, G. Hummer, and C. Dellago, "A one-dimensional dipole lattice model for water in narrow nanopores ", *Journal of Chemical Physics* **130**, 154110 (2009).

95. W. Lechner and C. Dellago, "Defect interactions in two-dimensional colloidal crystals: vacancy and interstitial strings", *Soft Matter* **5**, 2752 (2009).

96. M. Grünwald and C. Dellago, "Transition state analysis of solid-solid transformations in nanocrystals", *Journal of Chemical Physics* **131**, 164116 (2009).

97. J. Köfinger and C. Dellago, "Orientational dynamics and dielectric response of nanopore water", *Physical Review Letters* **103**, 080601 (2009).

98. T. Bucko, L. Benco, O. Dubay, C. Dellago, J. Hafner, "Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: ab-initio transition path sampling", *Journal of Chemical Physics* **131**, 214508 (2009).

99. P. Geiger and C. Dellago, "Optimum protocol for fast switching free energy calculations", *Physical Review E* **81**, 021127 (2010).

100. P. Geiger and C. Dellago, "Identifying rare chaotic and regular trajectories in dynamical systems with Lyapunov weighted path sampling", *Chemical Physics* **375**, 309 (2010).

101. E. Schöll-Paschinger and C. Dellago, "Demixing of a binary symmetric mixture studied with transition path sampling", *Journal of Chemical Physics* **133,** 104505 (2010).

102. H. Bosetti, H. A. Posch, C. Dellago, and W. G. Hoover, "Time-reversal symmetry and covariant Lyapunov vectors for simple particle models in and out of equilibrium", *Physical Review E* **82**, 046218 (2010).

103. J. Köfinger and C. Dellago, "Single-file water as a one-dimensional Ising model", *New Journal of Physics* **12**, 093044 (2010).

104. E. E. Borrero and C. Dellago, "Overcoming barriers in trajectory space: mechanism and kinetics of rare events via Wang-Landau enhanced transition path sampling", *Journal of Chemical Physics* **133**, 134112 (2010).

105. J. Köfinger and C. Dellago, "Microscopic properties of nanopore water from its time-dependent dielectric response", *Physical Review B* **82**, 205416 (2010). (Also published in the *Virtual Journal of Nanoscale Science & Technology*, Vol. 21, Issue 22, November 15, 2010).

106. M. Weinwurm and C. Dellago, "Vibrational Spectroscopy of Water in Narrow Nanopores", *Journal of Physical Chemistry B* **115**, 5268 (2011).

107. S. Jungblut and C. Dellago, “Crystallization of a binary Lennard-Jones mixture”, *Journal of Chemical Physics* **134**, 104501 (2011).

108. W. Lechner, C. Dellago and P. G. Bolhuis, “Role of the prestructured surface cloud in crystal nucleation”, *Physical Review Lett*ers **106**, 085701 (2011). *Selected as Editor’s Suggestion.*

109. E. E. Borrero, M. Weinwurm and C. Dellago, “Optimizing transition interface sampling simulations”, *Journal of Chemical Physics* **134**, 244118 (2011).

110. W. Lechner, C. Dellago, and P. G. Bolhuis, “Reaction Coordinates for the Crystal Nucleation of Colloidal Suspensions Extracted from the Reweighted Path Ensemble”, *Journal of Chemical Physics* **135**, 154110 (2011).

111. J. Köfinger, G. Hummer, and C. Dellago, “Single-file water in narrow, apolar pores”, *invited Perspective Article featured on the cover*, *Physical Chemistry Chemical Physics* **13, 15403** (2011).

112. S. Jungblut and C. Dellago, “Heterogeneous crystallization on tiny clusters”, *Europhysics Letters* **96**, 56006 (2011).

113. I. Coluzza and C. Dellago, “The configurational space of colloidal patchy polymers with heterogeneous sequences”, special issue 8th Liquid Matter Conference, *J. Phys.: Cond. Mat.* **24,** 284111 (2012).

114. G. Menzl, J. Köfinger and C. Dellago, “Phase transition and inter-pore correlations of water in nanopore membranes”, *Physical Review Letters* **109**, 020602 (2012).

115. M. Grünwald, S. Jungblut, and C. Dellago, “Transition Path Sampling for Materials – Nucleation in Materials hard and soft”, Lecture Notes for the Winter School on *Hierarchical Methods for Dynamics in Complex Molecular Systems*, Institute for Advanced Computing, Jülich Supercomputing Center, 5-9 March 2012; AIS-Series Volume **10**, 47 (2012).

116. D. Chandler, C. Dellago, and P. L. Geissler, “Wired-up water”, invited *News & Views* article, *Nature Chemistry* **4**, 245 (2012).

117. C. Dellago, G. Kahl, and C. N. Likos, „Preface: The Eighth Liquid Matter Conference“, *Journal of Physics: Condensed Matter* **24**, 280301 (2012).

118. C. Dellago, G. Kahl, and C. N. Likos, „Narrative: The Eighth Liquid Matter Conference“, *Journal of Physics: Condensed Matter* **24**, 280401 (2012).

119. A. Ballard and C. Dellago, “Towards the mechanism of ionic dissocation in water”, *Journal of Physical Chemistry B* **116**, 13490–13497 (2012).

120. Ivan Coluzza, Peter van Oostrum, Barbara Capone, Erik Reimhult, and Christoph Dellago, “Design and Folding of Colloidal Patchy Polymers”, *Soft Matter* **9, 938-944** (2013).

121. I. Coluzza, P. van Oostrum, B. Capone, E. Reimhult, and C. Dellago, „Sequence controlled self-knotting colloidal patchy polymers“, *Physical Review Letters* **110**, 075501 (2013).

122. S. Jungblut and C. Dellago, “Crystallization on pre-structured seeds“, *Physical Review E*, **87**, 012305 (2013).

123. P. E. Theodorakis, C. Dellago, and G. Kahl, “A coarse-grained model for DNA-functionalized spherical colloids, revisited: Effective pair potential from parallel replica simulations”, *Journal of Chemical Physics* **138**, 025101 (2013).

124. Q. Zhou, B. Wang, P. Wang, C. Dellago, Y. Wang, and Y. Fang, "Nanoparticle-Based Crystal Growth via Multistep Self-Assembly", *CrystEngComm* **15**, 5114 (2013).

125. J. Hasnain, S. Jungblut, and C. Dellago, "Dynamic phases of colloidal monolayers sliding on commensurate substrates", *Soft Matter* **9**, 5867 (2013). This research was featured in the cover of *Soft Matter*, July 10, 2013, Issue 25.

126. U. R. Pedersen, F. Hummel, G. Kresse, G. Kahl, and C. Dellago, "Computing Gibbs free energy differences by interface pinning", *Physical Review B* **88**, 094101 (2013).

127. C. Vogler, F. Bruckner, B. Bergmair, T. Huber, D. Suess, and C. Dellago, „Simulating rare switching events of magnetic nanostructures with forward flux sampling", *Physical Review B* **88**, 134409 (2013).

128. W. Lechner, D. Polster, G. Maret, P. Keim, and C. Dellago, "Self-organized defect strings in two-dimensional crystals", *Physical Review E* **88**, 060402 (2013).

129. S. Jungblut, A. Singraber, and C. Dellago, "Optimizing reaction coordinates for crystallization by tuning the crystallinity definition", *Molecular Physics* **111**, 3527-3533 (2013).

130. P. Geiger and C. Dellago. "Neural networks for local structure detection in polymorphic systems", *Journal of Chemical Physics* **139** , 164105 (2013).

131. C. Dellago and G. Hummer, "Computing equilibrium free energies using non-equilibrium molecular dynamics", *Entropy* **16**, 41-61 (2014).

132. J. Gieseler, R. Quidant, C. Dellago and L. Novotny, „Dynamic Relaxation of a Levitated Nanoparticle from a Non-Equilibrium Steady State", *Nature Nanotechnology* **9,** 358-364 (2014). doi:10.1038/nnano.2014.40. A news and views article about this work appeared in Nature Nanotechnology: Sergio Ciliberto, „On the way to equilibrium", *Nat. Nanotech*. **9**, 334 (2014).

133. P. Geiger, C. Dellago, M. Macher, C. Franchini, G. Kresse, J. Bernard, and T. Loerting, "Proton ordering of cubic ice Ic: experiments and computer simulations", *Journal of Physical Chemistry C* **118**, 10989 (2014). DOI:10.1021/jp500324x

134. J. Hasnain, S. Jungblut, A. Tröster, and C. Dellago, "Frictional dynamics of stiff monolayers: From nucleation dynamics to thermal sliding", *Nanoscale, **6**, 10161* (2014). DOI: 10.1039/C4NR01790K

135. M.A. Gonzalez, G. Menzl, J.L. Aragones, P. Geiger, F. Caupin, J. L. F. Abascal, C. Dellago, and C. Valeriani, "Detecting vapour bubbles in simulations of metastable water", *Journal of Chemical Physics* **141** , 18C511 (2014).

136. C. Leitold, and C. Dellago, „Folding mechanism of a polymer chain with short-range attractions", *Journal of Chemical Physics* **141**, 134901 (2014).

137. C. Vogler, B. Bergmair, F. Bruckner, T. Huber, D. Suess, C. Dellago, „Calculating thermal stability and attempt frequency of advanced recording structures without any free parameters", *Journal of Applied Physics* **117**, 163907 (2015).

138. U. R. Pedersen, F. Hummel, and C. Dellago, “Computing the crystal growth rate by the interface pinning method”, *Journal of Chemical Physics* **142**, 044104 (2015).

139. S. Jungblut and C. Dellago, "Caveats of mean first-passage time methods applied to the crystallization transition: effects of non-Markovianity", *Journal of Chemical Physics* **142**, 064103 (2015).

140. W. Lechner, D. Polster, G. Maret, C. Dellago, and P. Keim, "Entropy and kinetics of point defects in two-dimensional dipolar crystals", *Physical Review E* **91**, 032304 (2015).

141. J. Hasnain, S. Jungblut, C. Dellago, „Dynamical phases of attractive particles sliding on a structured surface“, *Journal of Physics Condensed Matter* **27**, 194122 (2015).

142. C. Leitold, W. Lechner, and C. Dellago, „A string reaction coordinate for the folding of a polymer chain“, *Journal of Physics Condensed Matter* **27**, 194126 (2015).

143. J. Gieseler, L. Novotny, C. Moritz, and C. Dellago, "Non-equilibrium steady state of a driven levitated particle with feedback cooling", *New Journal of Physics* **17***,* 045011 (2015). *Invited article for special issue on stochastic thermodynamics.*

144. P. Wirnsberger, D. Frenkel, and C. Dellago, „An enhanced version of the heat exchange algorithm with excellent energy conservation properties“, *Journal of Chemical Physics* 143, 124104 (2015). *Selected for the 2015 JCP Editor’s Choice Selection.*

145. P. G. Bolhuis and C. Dellago, "Practical and conecptual path samplig issues", *European Journal of Physics – Special Topics* **224**, 1-19 (2015).

146. P. E. Theodorakis, N. G. Fytas, G. Kahl, and C. Dellago, „Self-assembly of DNA-functionalized Colloids", *Condensed Matter Physics* **18**, 22801 (2015).

147. S. Jungblut and C. Dellago, „On the reaction coordinate for seeded crystallization“, *Molecular Physics* **113**, 2735 (2015). Invited article for the special issue for J.-P. Hansen.

148. T. Morawietz, A. Singraber, C. Dellago, and J. Behler, „How Van der Waals interactions determine the unique properties of water“, *Proc. Natl. Acad. Sci. USA* **113**, 8368-8373 (2016).

149. S. Jungblut and C. Dellago, „Pathways to self-assembly: crystallization by nucleation and growth“, *Lecture Notes of the Enrico Fermi School on Soft Matter Self-Assembly*, in print (2016). Also published in *European Physical Journal E* **39**, 77 (2016).

150. P. Wirnsberger, D. Fijan, A. Šarić, M. Neumann, C. Dellago and D. Frenkel, „Non-equilibrium simulations of thermally induced electric fields in water“, *Journal of Chemical Physics* **144**, 224102 (2016).

151. G. Menzl, M.A. Gonzalez, P. Geiger, F. Caupin, J.L.F. Abascal, C. Valeriani, and C. Dellago, “Molecular mechanism of cavitation in water under tension”, *Proc. Natl. Acad. Sci. USA* **113**, 13582-13587 (2016). DOI 10.1073/pnas.1608421113. A commentary of our article appeared in the same issue of PNAS: D. Lohse and A. Prosperetti, "Homogeneous

nucleation: Patching the way from the macroscopic to the nanoscopic description", *Proc. Natl. Acad. Sci. USA* **113**, 13549-13550 (2016). DOI 10.1073/pnas.1616271113

152. V. Jain, J. Gieseler, C. Moritz, C. Dellago, R. Quidant, and Lukas Novotny, „Direct Measurement of Photon Recoil from a Levitated Nanoparticle“, *Phys. Rev. Lett.* **116**, 243601 (2016).

153. E. E. Borrero and C. Dellago, “Avoiding traps in trajectory space: metadynamics enhanced transition path sampling”, *European Physical Journal Special Topics* **225**, 1609-1620 (2016). Invited article for the Festschrift for K. Kremer. DOI: 10.1140/epjst/e2016-60106-y

154. G. Menzl, A. Singraber, and C. Dellago, “S-shooting: a Bennett-Chandler method for the calculation of reaction rate constants from committor trajetories”, Faraday Discusssions **195**, 345-364 (2016). DOI: 10.1039/C6FD00124F

155. G. Menzl and C. Dellago, “Effect of entropy on the nucleation of cavitation bubbles in water under tension”, invited article for special issue on nucleation, *Journal of Chemical Physics,* **145**, 211918 (2016). http://dx.doi.org/10.1063/1.4896560

156. C. Leitold and C. Dellago, “Nucleation dynamics and structural growth of cluster crystals”, *Journal of Chemical Physics,* **145**, 074504 (2016). DOI: 10.1063/1.4960958

157. S. Jungblut and C. Dellago, “Heterogeneous Crystallization on pairs of pre-structured seeds”, *Journal of Physical Chemistry B* **120**, 9230-9239 (2016). DOI: 10.1021/acs.jpcb.6b06510

158. V. Bianco, G. Franzese, C. Dellago, and I. Coluzza “The role of water in the selection of stable proteins at ambient and extreme thermodynamic conditions", *Physical Review X* **7**, 021047 (2017).

159. C. Cardelli, V. Bianco, L. Rovigatti, C. Dellago and I. Coluzza, “The role of directional interactions in the designability of generalized heteropolymers”, *Scientific Reports* **7**, 4986 (2017). DOI: 10.1038/s41598-017-04720-7

160. Ivan Coluzza, Jessie Creamean, Michel Rossi, Heike Wex, Peter Aaron Alpert, Valentino Bianco, Yvonne Boose, Christoph Dellago, Laura Felgitsch, Janine Fröhlich, Hartmut Herrmann, Swetlana Jungblut, Zamin Kanji, Georg Menzl, Bruce Moffett, Clemens Moritz, Anke Mutzel, Ulrich Pöschl, Michael Schauperl, Jan Scheel, Emiliano Stopelli, Frank Stratmann, Hinrich Grothe, and David G. Schmale III, “Perspectives on the Future of Ice Nucleation Research: Unanswered Questions and Research Needs Identified from Two International Workshops”, *Atmosphere* **8**, 138 (2017). DOI: 10.3390/atmos8080138

161. P. Wirnsberger, D. Fijan, R. Lightwood, A. Šarić, C. Dellago, and D. Frenkel, “Numerical Evidence for Thermally Induced Monopoles”, *Proc. Natl. Acad. USA* **114**, 4911-4914 (2017). DOI: 10.1073/pnas.1621494114

162. L. Rondin, J. Gieseler, R. Quidant, C. Dellago, and L. Novotny, "Direct Measurement of Kramers' Turnover with a Levitated Nanoparticle", *Nature Nanotechnology*, advance online publication (2017). doi:10.1038/nnano.2017.198. A "News & Views" commentary on our article appeared in the same issue: Nikolai Kiesel and Eric Lutz , "Nanoparticles jumping high", *Nature Nanotechnology*, advance online publication (2017)doi:10.1038/nnano.2017.219

163. J. Hasnain, S. Jungblut, G. Menzl, and C. Dellago, "Crystallization and flow in active patch systems", *Soft Matter* **13**, 930-936 (2017). DOI: 10.1039/C6SM01898J

164. M. Sega and C. Dellago, "Long-range dispersion effects on the water/vapor interface simulated using the most common models", *Journal of Physical Chemistry* **121**, 3798-3803 (2017). Contribution for the Memorial Issue of Klaus Schulten. DOI: 10.1021/acs.jpcb.6b12437

165. C. Moritz, A. Tröster, and C. Dellago, "Geometric phase transitions in systems with periodic boundary conditions", *Journal of Chemical Physics* **147**, 152714 (2017). DOI: 10.1063/1.4997479

167. Max Burian, Carina Karner, Maksym Yarema, Wolfgang Heiss, Heinz Amenitsch, Christoph Dellago, and Rainer T. Lechner, "Shape induced orientation phase within 3D nanocrystal solids", *Advanced Materials*, submitted (2018).

168. Erik Hebestreit, Martin Frimmer, René Reimann, Christoph Dellago, Francesco Ricci and Lukas Novotny, "Calibration and temperature measurement of levitated optomechanical sensors", *Review of Scientific Instruments*, submitted (2018).

169. C. Karner and C. Dellago, "Non-classical freezing of hard cube colloids", submitted to Phys. Rev. Lett. (2018).

170. G. Menzl, D. Donadio, R. Scipioni, L. M. Ghiringhelli, L. Delle Site, and C. Dellago, "Proton transport along water wires adsorbed on stepped metal surfaces", in preparation (2018).

171. C. Tung, M. Grünwald and C. Dellago, "Tuning nucleus morphology and transformation mechanisms in lattice models of nanocrystals", in preparation (2018).

172. E. E. Borrero, M. Weinwurm and C. Dellago, "Optimized transition interface sampling for simulations of rare events: II. Kinetic mechanism and reaction coordinates estimates", in preparation (2018).

Lectures, Seminars, Talks

1. *Lyapunov instability of the XY-model*, CECAM Workshop "Chaotic and ordered energy flow in lattices", Lyon, France, August 29 - September 9, 1994.
2. *Kolmogorov-Sinai entropy and Lyapunov spectra of a hard sphere gas*, CECAM Euroconference "The Microscopic Approach to Complexity by Molecular Simulations", Lyon, France, July 15-19, 1996.

3. *Simulating rare events in complex systems by transition path sampling*, Department of Chemistry, MIT, Boston, Massachusetts, January 19, 1998.
4. *Finding reaction mechanisms and calculating rate constants with transition path sampling*, Department of Chemistry, Cambridge University, Cambridge, UK, May 15, 1998.
5. *Simulating rare events in complex systems by transition path sampling*, Department of Chemistry, Rice University, Houston, Texas, November 23, 1998.
6. *Simulating rare events in complex systems by transition path sampling*, Department of Chemistry, University of Rochester, Rochester, New York, December 8, 1998.
7. *Simulating rare events with transition path sampling*, Los Alamos National Laboratory, Los Alamos, New Mexico, December 23, 1998.
8. *Simulating rare events in complex systems by transition path sampling*, EMLG Annual Conference 1998: "PHYSICS OF LIQUIDS: FOUNDATIONS, HIGHLIGHTS, CHALLENGES", Murau, Austria, September 11-16, 1998.
9. *Studying rare events with transition path sampling*, Computational Chemistry Seminar, February 25, 1999, Department of Chemical Engineering, University of Amsterdam, The Netherlands, February 26, 1999.
10. *Transition Path Sampling and its Applications*, four lectures, CECAM Tutorial on Transition Path Sampling, Lyon (France), October 18-22, 1999.
11. *The kinetics of ion pair dissociation in water: a transition path sampling study*, Condensed Matter Physics Seminar, Department of Physics, University of Rochester, Rochester, NY, November 8, 1999.
12. *Proton transfer in aqueous environments: from clusters to liquids*, Pitzer Memorial Symposium on Theoretical Chemistry, Berkeley, California (USA), January 9-13, 2000.
13. *Charge separation in aqueous environments studied with transition path sampling*, Statistical Mechanics Seminar, Department of Chemistry, Cornell University, Ithaca, NY, April 7, 2000.
14. *Kinetics of charge separation in aqueous solution*, Chemical Physics Seminar, NIH, Washington D.C, April 20, 2000.
15. *Studying rare events with transition path sampling: methods and applications*, Chemical Physics Seminar, NIH, Washington D.C, April 20, 2000.
16. *Transition path sampling study of autoionization of water*, CECAM-SIMU Workshop 'Simulations of Long Time Scale Dynamics: Molecular and Continuum Descriptions', Reykjavik, Iceland, June 25-30, 2000.
17. *Charge separation in aqueous environments studied with transition path sampling*, Workshop on Condensed Phase Dynamics, Telluride Summer Research Center, Telluride, CO, July 24, 2000.
18. *Autodissociation of a water molecule in liquid water*, Symposium on 'Proton Transport in Liquids, Solids and Proteins', 220th National Meeting of the ACS, Washington DC, August 20-24, 2000.

19. *Charge separation in aqueous environments studied with transition path sampling*, Institute for Physical Science and Technology, University of Maryland, College Park, MD, September 20, 2000.

20. *Exploring Complex Systems with Computer Simulation*, Department of Chemistry, St. John Fisher College, Rochester, NY, November 17, 2000.

21. *Proton transport in aqueous environments*, Department of Chemistry, University of Toronto, Toronto, March 13, 2001.

22. *Autoionization in liquid water*, International Conference on Computational Nanoscience, Hilton Head, SC, March 19-21, 2001.

23. *Autoionization in liquid water and proton transport in aqueous environments*, Department of Chemistry, University of Chicago, Chicago, USA, April 30, 2001.

24. *Proton transport in water*, Gordon Conference 'Chemistry and Physics of Liquids', Holderness School, NH, August 5-10, 2001.

25. *Exploring Complex Systems with Transition Path Sampling,* Conference on 'Bridging the time-scale gap' of the SIMU programme, Konstanz, Germany, September 10-13, 2001.

26. *Proton transfer through a water filled Carbon nanotube*, Gordon Conference 'Water and Aqueous Solutions', Holderness School, NH, August 4-9, 2002.

27. *Proton transfer through a water filled Carbon nanotube*, Berkeley Mini Statistical Mechanics Meeting 2003, Berkeley, CA, January 10-12, 2003.

28. *Proton transfer through water filled pores*, ASPUS (Applied Statistical Physics and Simulation) Seminar Series, Institute for Experimental Physics, University of Vienna, Vienna, April 2, 2003.

29. *Out of equilibrium in trajectory space*, Workshop on 'Metastability and landscapes in complex system', CECAM, Lyon, France, May 22-24, 2003.

30. *Calculating time correlation functions by changing ensembles of trajectories*, Conference on 'The Monte Carlo Method in the Physical Sciences: Celebrating the 50th anniversary of the Metropolis algorithm', Los Alamos, New Mexico, June 9-12, 2003.

31. *Exploring Complex Systems with Transition Path Sampling*, Computational Materials Science Seminar, Institute for Materials Physics, University of Vienna, June 23, 2003.

32. *Out of equilibrium in trajectory space*, Workshop on 'Multiscale Modelling of Chemical Reactions", CECAM, Lyon, France, September 3-5, 2003.

33. *Computational Physics - Ein Streifzug von harten Kugeln zu weicher Materie*, Antritts-vorlesung am Institut für Experimentalphysik der Universität Wien, 16. Dezember 2003.

34. *Studying Rare Events in Complex Systems*, Workshop „Progress in Ab Initio Computational Methods for Condensed Matter", Gif sur Yvette, France, 9. Jänner 2004.

35. *Simulating Rare Events with Transition Path Sampling*, eingeladener Vortrag, Freie Universität Berlin, Fachbereich Mathematik + Informatik, Numerische Mathematik /Scientific Computing, Berlin, Deutschland, 13. Februar 2004.

36. *Proton Transport through Water-Filled Carbon Nanotubes*, Seminarvortrag an der Universität der italienischen Schweiz (Prof. Michele Parrinello), Lugano, Schweiz, 6. April 2004.

37. *Proton transport through water-filled pores*, Seminarvortrag am Physikalisch-Chemischen Institut der Universität Zürich, Zürich, Schweiz, 29. April 2004.

38. *Warum ist Wasser naß?* Vortrag im Rahmen der Führung von Gymnasialklassen durch Arbeitsgruppen des Instituts für Experimentalphysik der Universität Wien, 26. Mai 2004.

39. *Biased sampling of non-equilibrium trajectories: Can fast switching simulations beat conventional free energy calculation methods?,* CECAM (European Centre for Atomic and Molecular Computations) in Lyon, Frankreich, 23. Juni 2004.

40. *Rate constants via transition path sampling*, CECAM -Workshop „Conformational Dynamics in Complex Systems“, in Lyon, Frankreich, 16. Juli 2004.

41. *Path sampling of fast switching trajectories,* CECAM-Workshop „Conformational Dynamics in Complex Systems“, in Lyon, Frankreich, 16. Juli 2004.

42. *Biased Sampling of non-equilibrium trajectories: Can fast switching simulations beat conventional free energy calculation methods?*, SIMU Conference: Bridging the Scales (29.-31. August 2004) Genua, Italien, 30. August 2004.

43. *Proton Transport through Water-Filled Carbon Nanotubes*, Conference on Computational Physics 2004 (1.-4. September 2004), Genua, Italien, 2. September 2004.

44. *Proton Transport through Carbon Nanotubes*, Jahrestagung der Österreichischen Physikalischen Gesellschaft, Fachausschuß Festkörperphysik, Linz, 28. September 2004.

45. *Computational Physics an der Universität Wien*, Rotary Club Wien-Donau, Hotel de France, 6. Oktober 2004.

46. *Rare events in complex systems: from chemical reactions to nucleation*, Universität Wien, wöchentliches Seminar der Aerosolgruppe, 29. Oktober 2004.

47. *Rare events in trajectory space*, The 2005 Berkeley Mini Statistical Mechanics Meeting marking David Chandler’s 60th birthday, (January 7-9, 2005), Berkeley, USA, January 7, 2005.

48. *Exploring complex systems with transition path sampling*, Literaturseminar, Universität Wien, Institut für Theoretische Physik, Wien, January 13, 2005.

49. *Exploring complex systems with transition path sampling*, Universität Bonn, January 20, 2005.

50. *Biased sampling of non-equilibrium trajectories: Can fast switching simulations beat conventional free energy calculations?*, Max-Planck Institut Mainz, January 25, 2005.

51. *Exploring complex dynamics with transition path sampling,* 69. Tagung der Deutschen Physikalischen Gesellschaft (DPG), 4-9 March 2005, Berlin, March 8, 2005.

52. *Rare events in complex systems: from chemical reactions to the nucleation of phase transitions*, Vortrag im Rahmen der Seminarreihe „Order and disorder in complex systems“, Institute for Experimental Physics, University of Vienna, 26 April 2005.

53. *Proton transfer through narrow pores*, Universität Amsterdam, The Netherlands, 28 April, 2005.

54. *Some computational aspects of the Jarzynski identity*, FOM Institute for Atomic and Molecular Physics - AMOLF, Amsterdam, The Netherlands, April 29, 2005.

55. *Reaction kinetics from transition path sampling simulations,* Workshop „Conformational dynamics in complex systems“, CECAM Lyon, France, 5 - 10 June 2005.

56. *Transition path sampling methods*, International School of Solid State Physics, Erice, Sicily, 20 - 26 July 2005.

57. *Rare events in complex systems: from chemical reactions to the nucleation of phase transitions*, Meeting of the International Board, Center for Computational Material Science - CMS, November 18, 2005.

58. *Good equilibrium free energies from bad non-equilibrium dynamics*, Poster, Berkeley Mini Statistical Mechanics Meeting, University of California, Berkeley, USA, 13 - 15 January 2006.

59. *The Jarzynski identity as a computational tool*, University of California at Irvine, USA, 12 January 2006.

60. *The Jarzynski identity as a computational tool*, International Conference „Work, Dissipation, and Fluctuations in Nonequilibrium Physics“, Université Libre de Bruxelles, Brussels, Belgium, 22 - 25 March 2006.

61. *Bridging the time scale gap in molecular simulations,* Conference of the The Royal Netherlands Academy of Arts and Sciences „Multiscale modelling: electrons, molecules and (bio)material“, 3-5 April 2006, Amsterdam, The Netherlands, 4 April 2006. ivited lecture

62. *From hard spheres to soft matter: Boltzmann's legacy for the computational physicist,* International Symposium in Commemoration of Ludwig Boltzmann's Death on September 5, 1906, Erwin Schrödinger Institute for Mathematical Physics, Vienna, Austria, 8 June 2006.

63. *Transition path sampling studies of phase transition*, Seventh Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, 14 June 2006.

65. *Good equilibrium free energies from bad non-equilibrium trajectories*, CECAM workshop "Theory of single molecule force experiments and simulations", Lyon, France, 27 September 2006.

66. *Studying phase transitions with transition path sampling***,** University of Cambridge, 19-23 November 2006.

67. *Transition path sampling: simulating rare events in complex systems*, "SimBioMa Workshop on Path Sampling in Molecular Simulation Paris", Paris, Frankreich, 29 November 2006.

68. *Exploring Complex Dynamics with Transition Path Sampling***,** Seminarvortrag in der Gruppe Prof. Wolfgang Domcke, Lehrstuhl für Theoretische Chemie, Technische Universität München, 19 December 2006.

69. *Transition path sampling studies of phase transitions*, 2007 March Meeting of the American Physical Society, March 5-9, 2007 in Denver, Colorado, USA, 2007.

70. *Phase transformations and transition path sampling methods,* lecture at the Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin, 26 April 2007.

71. *Phase transformations and transition path sampling methods*, CCP 2007 - Conference on Computational Physics, Brussels, Belgium, 5-8 September 2007.

72. *Some computational aspects of the Jarzynski identity,* Conference "Non-Equilibrium Steady States", Paris, 8-12 October 2007.

73. *Studying phase transformations with transition path sampling,* Ruhr-Universität Buchum (Prof. Marx), Bochum, Gemany, 7 November 2007.

74. *Defect Interactions in Colloidal Crystals*, Berkeley Mini Statistical Mechanics Meeting, Berkeley, USA, 11 - 13 January 2008.

75 *Studying phase transformations with transition path sampling*, Conference Metastability and Rare Events in Complex Systems, The Erwin Schrödinger International Institute for Mathematical Physics, Wien, 13 February 2008.

76. *Proton transport through water-filled narrow pores*, DPG Frühjahrstagung - Symposium Computational Soft matter physics (SYMP), Berlin, 28 February 2008.

77. *Physik an der Universität Wien studieren: Motivationen und Möglichkeiten"*, BESt^3 - Die Messe für Beruf, Studium und Weiterbildung, veranstaltet vom BM für Unterricht, Kunst und Kultur und dem Arbeitsmarktservice Österreich, Wiener Stadthalle, 6 March 2008.

78. *Interactions and dynamics of defects in colloidal crystals*, International Conference "Colloidal Dispersions in External Fields - CODEF II" , Bonn, Germany, 31 March 2008.

79. *Computer Simulation of Nanoparticles under Pressure*, Poster: M.Grünwald, C. Dellago, SimBioMa 2008 - Conference on Molecular Simulatiuons in Biosystems and Material Science, University of Konstanz, Germany, 2-5 April 2008.

80. *Macroscopically Ordered Water in Nanopores*, Poster: J. Köfinger, C. Dellago, 33rd Conference of the Middle European Cooperation in Statistical Physics - MECO33, Puchberg/Wels, Austria, 14-16 April 2008.

81. *Some computational aspects of the Jarzynski identity*, Seminar talk - Seminar of Statistical Physics, Institute de Physique Theorique, CEA, Saclay, France, 19.5.2008.

81. *Summer School "Progress in Simulating Activated Processes",* May 26-30, 2008, Valle Capore, Italy. Titles of the lectures: 1) Transition State Theory, 2) Transition Path Sampling, 3) Path Analysis: Finding the Mechanism, 4) Kinetics from Transition Path Sampling, 5) Rare Events in Path Space: Non-equilibrium Fast Switching. Invited lectures

82. *Bridging time scales in molecular simulations: Phase transformation in nanoparticles*, The Amsterdam Center for Multiscale Modelling (ACMM) Opening Symposium, June 26, 2008, Amsterdam, The Netherlands.

83. *Atomistische Simulation: Materialforschung im virtuellen Labor*, Universitätstag "Grenzgänge der Materialwissenschaft, Europäisches Forum Alpbach, 23.-24.8.2008, Alpbach, Austria.

83. *Path Sampling*, 5th MATCOR summer school of the Graduate School Mainz-"Simulation of Macromolecules on different Scales", Hall in Tirol, Austria, August 31-September 5, 2008. (gehalten September 5th) .

84. *Pressure induced phase transformations on nanocrystals studied with transtition path sampling simulations ,* IK and NFN tutorial and discussion meeting "Multiscale phenomena in materials" , September 10-12, 2008, Vienna , Austria.

85. *Pressure induced phase transformations of nanocrystals studied with transition path sampling simulations,* E-MRS Fall Meeting, September 15-19 , 2008, Warsaw, Poland.

86. *The unusual properties of water in narrow pores,* Awards Ceremony of the Gutenberg Lecturer Award 2008, October 21, 2008, Mainz, Germany.

87. *Simulating rare events in complex systems: from transition state theory to transition path sampling,* Fall School on “Biomolecules: Physical Principles and Mechanisms”, November 3, 2008, Prague, Czech Republic.

88. *Analyzing transition pathways: mechanism and rate constants,* Fall School on “Biomolecules: Physical Principles and Mechanisms”, November 3, 2008, Prague, Czech Republic.

89. *Precision Shooting: sampling long, diffusive trajectories*, Workshop: “Molecular Dynamics, Thermostats and Convergence to Equilibrium”, November 12, 2008, Edinburgh, Scotland.

90. *Parallel computing in molecular dynamics and Monte Carlo simulations*, Workshop: “Computational Science and Engineering (CSE 2009)”, January 09, 2009, Rust, Austria.

91. *Pressure induced phase transformations of nanocrystals studied with transition path sampling simulations*, Physikalische Chemie-Kolloquium Frühjahrssemester 2009, Laboratorium für Physikalische Chemie, ETH Zürich, March 03, 2009, Zürich, Switzerland.

92. *Water in narrow pores*, International workshop “From Structure to Function: Influx and Efflux Systems”, May 6-8, 2009, Cagliari, Sardinia, Italy.

93. *The time scale problem in molecular simulations*, May 20, 2009, Institute for Quantum Optics and Quantum Information, Vienna, Austria.

94. *Pressure induced phase transformations of nanocrystals studied with transition path sampling simulations*, Workshop “Catalysis from first principles – Cat1P”, Erwin Schrödinger Institute, 25-28 May, 2009, Vienna, Austria.

95. *Nucleation and growth in structural transformations of nanocrystals*, Workshop “Molecular Kinetics”, May 26-30, 2009, Berlin, Germany.

96. *Water in narrow pore*s, June 9-10, 2009, Max Planck Institut für Metallforschung, Stuttgart, Germany.

97. *Sampling and analysing rare nucleation pathways*, Workshop "Biomolecular Simulations: Advanced Methods and Applications", June 28-30, 2009, Karolinska Institutet, Stockholm, Sweden.

98. *Nucleation and growth in nanocrystals: insights from transition path sampling simulations*, Workshop CECAM: "Structural Transitions in solids: theory, simulations, experiments and visualisation Techniques", July 8-11, 2009, Lugano, Schweiz.

99. *Water in narrow pores*, “XIII European Conference on the Spectroscopy of Biological Molecules”, August 28-September 2, 2009, Palermo, Italy.

100. *Water in narrow pores*, Conference „EMLG-JMLG Annual Meeting 2009 - Intermolecular Interactions and Liquid Structure”, September 6-10, 2009, Salzburg, Austria.

101. *Bridging time scales in molecular simulations: from nanocrystals to colloidal suspensions*, Workshop CompMat´09, October 1-2, 2009, Stadt Schlaining, Austria.

102. *Computer simulation of nucleation phenomena: pressure-induced structural transformations in nanocrystals*, Conference “Complex Energy Landscapes and Long Time Scales”, November 11-14 2009, Princeton University, USA.

103. *Computational Physics: Das virtuelle Labor im Supercomputer*, Schülervortrag am Bundesgymnasium und Bundesrealgymnasium mit besonderer Berücksichtigung der musischen Ausbildung, Boerhaavegasse 15, 1030 Wien, Novermber 26, 2009.

104. *Sampling rare chaotic and regular trajectories*, Conference „Mini Statistical Mechanics Meeting“ - Special Session on Transition Path Sampling, University of California at Berkeley, Berkeley, USA, January 8-10, 2010.

105. *Water in narrow pores*, Conference "Mini Statistical Mechanics Meeting", University of California at Berkeley, Berkeley, USA, January 8-10, 2010.

106. *The time scale problem in molecular simulation*, ÖFG Workshop „High Performance Computing 2010“, Technical University of Vienna, Vienna, Austria, February 18-19, 2010.

107. *Physik an der Uni Wien studieren: Möglichkeiten und Motivationen*, BESt^3 - Die Messe für Beruf, Studium und Weiterbildung, veranstaltet vom BM für Unterricht, Kunst und Kultur, dem BM für Wissenschaft und Forschung, und dem Arbeitsmarktservice Österreich, Wiener Stadthalle, March 6, 2010.

108. *The time scale problem im molecular simulation: nucleation of of first order phase transitions*, Seminar of VERA (Vienna environmental research accelerator), Isotope Physics Group, Faculty of Physics, University of Vienna, March 11, 2010.

109. *The time scale problem in molecular simulations: pressure-induced structural transformations in nanocrystals,* Seminar talk at the Department of Physics, University of Ljubljana and Jozef Stefan Institute, Ljubljana, Slovenia, April 19, 2010.

110. *Computational Physics: Das virtuelle Labor im Supercomputer*, Festvortrag bei Preisverleihung Physikolympiade, Wiedner Gymnasium, Wien, April 21, 2010.

111. *Pressure-induced structural transformations in nanocrystals,* Seminar of the Theory Group, Max-Planck-Institute fpr Polymer Research, Mainz, Germany, April 27, 2010.

112. *Water in narrow pores*, Condensed Matter Physics Seminar, Weitzmann Institute, Rehovot, Israel, Mai 12, 2010.

113. *The time scale problem in molecular simulations: pressure-induced structural transformations in nanocrystals*, Physik Kolloquium, Universität Augsburg, Germany, Mai 17, 2010.

114. *Nucleation in small systems*, Conference on “Multiscale Molecular Modeling”, Edinburgh, UK, 30 June – 3 July, 2010.

115. *Nucleation and growth in nanocrystals: insights from transition path sampling* (Poster), 23rd General Conference of the Condensed Matter Division of the European Physical Society, 30 August – 3 September, 2010, Warsaw, Poland.

116. *Nucleation in small systems*, Workshop “Novel Simulation Approaches to Soft Matter Systems”, 20-24 September, 2010, Dresden, Germany.

117. *Multiple time scales in the modeling of nucleation and growth: transition path sampling of pressure induced phase transitions in semiconductor nanocrystals*, ETH/CECAM/ESF Workshop in „Multiscale Modeling and Simulation“, 19-22 October, 2010, Kartause Ittingen, Switzerland.

118. *Local structure recognition with neural networks,* Kickoff-Meeting of the SFB Vienna Computational Materials Laboratory – ViCoM, 28-29 October, 2010, Burg Schlaining, Burgenland, Austria.

119. *Water in narrow pores: How orientational defects and protons move along 1d water wires,* BioScience 2010: Workshop on expanding the frontiers of biomolecular science, November 15-17, 2010, Forschungszentrum Jülich, Jülich, Germany.

120. *Nucleation in Small Systems: pressure induced phase transformations in nanocrystals,* Seminar talk at the Institute of Physics, University of Leoben, Leoben, Austria, November 23, 2010.

121. *Computational Physics: Das virtuelle Labor im Supercomputer*, Schülervortrag am Bundesgymnasium und Bundesrealgymnasium Wien 12, Rosasgasse 1-3, 1120 Wien, November 25, 2010.

122. *The Jarzynski equality and the Crooks fluctuation theorem: from the classical to the quantum regime*, Weekly Seminar of the Quantum Opto-Mechanics Group (Prof. Aspelmeyer), Faculty of Physics, University of Vienna, December 1, 2010.

123. *Phase transitions in nanocrystals: nucleation in small systems*, Workshop „Towards Reality in Nanoscale Materials '10", 6-8 December 2010, Levi, Finland.

124. *Nucleation in small systems: pressure induced phase transitions in nanocrystals*, Seminar talk at the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Bochum, Germany, January 31, 2011.

125. *Nucleation in small systems: Studying pressure induced phase transformations in nanocrystals studied with transition path sampling*, Computational Science Seminar, University of Basel, Basel, Switzerland, March 8, 2011.

126. *Water in Narrow Pores: How orientational defects and protons move along 1d water wires,* Physical Chemistry Seminar, University of Basel, Basel, Switzerland, March 9, 2011.

127. *Bridging time scales in molecular simulations: from nanocrystals to colloids,* Workshop Biomolecular Simulation in Vienna, Max F. Perutz Laboratories, University of Vienna, April 14, 2011.

128. *Nucleation in small systems: Studying pressure induced phase transformations in nanocrystals with transition path sampling*, Seminar Abteilung Jansen, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany, May 4, 2011.

129. *Simulating rare events with transition path sampling*, Joint Seminar on Complex Stochastic Systems, Medical University of Vienna and University of Vienna, Vienna, Austria, May 6, 2011.

130. *Computational Physics: the virtual laboratory in the supercomputer*, lecture for the student of the Janos Bolyai Gimnaszium (high school) in Szombathely, Hungary, May 11, 2011.

131. *Nucleation in small systems: Studying pressure induced phase transformations in nanocrystals with transition path sampling,* Seminar at the Faculty of Sciences, University of Western Hungary, Szombathely, Hungary, May 11, 2011.

132. *Challenges in the simulation of nucleation processes: from transition pathways to reaction coordinates*, Workshop "Catalysis from 1st Principles", Magleas, Denmark, May 22-26, 2011.

133. *The time scale problem in molecular simulations: from transition pathways to reaction coordinates*, Seminar of the Institute for Applied Statistics, University of Linz, Linz, Austria, June 9, 2011.

134. *Transition Path Sampling. Rare events: from transition pathways to reaction coordinates*, 2 lectures at the summer school "Modern Computational Science", University of Oldenburg, Oldenburg, Germany, August 15-26, 2011 (August 22, 2011).

135. *Challenges in the simulation of nucleation processes: from transition pathways to reaction coordinates*, 24th Marian Smoluchowski Symposium on Statistical Physics, Zakopane, Poland, September 17-22, 2011.

136. *Atomistic Simulation: Materials Science in the Virtual Laboratory*, Workshop of the Austrian Centre for Scientific Computing "Future Tools and Topics", University of Linz, Linz, Austria, October 17, 2011.

137. *Challenges in the simulation of nucleation processes: from transition pathways to reaction coordinates*, ZCAM (Zaragoza Scientific Center for Advanced Modelling), Zaragoza, Spain, February 23, 2012.

138. *Transition Path Sampling for Materials – Hard and Soft: Pathways to Nucleation and Growth,* IAS Winter School "Hierarchical Methods for Dynamics in Complex Molecular Systems", Forschungszentrum Jülich, Jülich, Germany, 5-9 March 2012.

139. *Transition Path Sampling. Rare events: from transition pathways to reaction coordinates,* Max F. Perutz Laboratories, University of Vienna, Vienna, Austria, May 15, 2012.

140. *Challenges in the simulation of nucleation processes: from transition pathways to reaction coordinates,* Workshop „Modeling Soft Matter: Linking Multiple Length and Time Scales", Kavli Institute of Theoretical Physics, University of California at Santa Barbara, Santa Barbara, USA, 4-8 June 2012. (The Workshop was part of the program „Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter" at the KITP.)

141. *Classifying local atomic structures with neural networks,* Highlight-Lecture at the Workshop "Modelling the Dynamics of Complex Molecular Systems", Lorentz Center, University of Leiden, Leiden, The Netherlands, 13-17 August 2012.

142. *Local Structure detection with neural networks*, CECAM Workshop "Machine Learning in Atomistic Simulations", USI, Lugano, Switzerland, 10-12 September 2012.

143. Multiscale *challenges in the simulation of nucleation and growth: from transition pathways to reaction coordinates,* Semi-plenary talk at the European Congress on Computational Methods in Applied Science and Engineering – ECCOMAS 2012, Vienna, Austria, 10-14 September, 2012.

144. *Nucleation and growth in small systems*, conference „Statistical Mechanics: Interplay of Theory and Computer Simulations" in honor of Kurt Binder, Mainz, Germany, 19-21 September 2012.

145. *Computational Physics: Das virtuelle Labor im Supercomputer*, Realgymnasium Parhamerplatz, 1170 Wien, November 14, 2012.

146. *Nucleation and growth at the nanoscale: from transition pathways to reaction coordinates*, Physics Department Colloquium (Seminaire General) of the Ecole Normale Superieure, Paris, France, November 29, 2012.

147. *Nucleation and growth at the nanoscale: from transition pathways to reaction coordinates*, Freiburg Institute for Advanced Studies (FRIAS), Freiburg, Germany, December 17, 2012.

148. *Nucleation at the nanoscale: pathways of phase transitions in small systems,* Workshop "Statistical, stochastic and related methods", University of Graz, Graz, Austria, April 10, 2013 .

149. *Phase transitions at the nanoscale: freezing/melting and structural changes in nanoparticles,* Seminar at the Department of Chemistry, Eötvös University, Budapest, Hungary, April 19, 2013 .

150. *Nucleation at the nanoscale: pathways of phase transitions in small systems,* Colloquium of the Department of Physics, Bilkent University, Ankara, Turkey, April 24, 2013 .

151. *Challenges in the simulation of nucleation processes: from transition pathways to reaction coordinates,* Charlemagne Lecture Series 2013, RWTH Aaachen, Germany, May 6, 2013.

152. *Neural networks for energy calculation and structure recognition***,** seminar at SISSA (Scoula Internazoinale di Studi Avanzati), Trieste, Italy, May 20, 2013.

153. *Nucleation at the nanoscale: Optimizing the definition of crystallinity***,** CECAM-Workshop „The role of interfaces in crystallization", Lausanne, Switzerland, 22-24 May, 2013.

154. *Attractive Imperfections: Defects in 2d crystals in equilibrium and non-equilibrium states***,** Seminar at the Department of Chemistry, University of Cambridge, Cambridge, UK, June 7, 2013.

155. *Neural networks for energy computation and structure recognition***,** Program on „Advanced Molecular Simulation Methods in the Physical Sciences", Kavli Institute for Theoretical Physics China, Beijing, China, June 24, 2013.

156. *Defects in colloidal monolayers in and out of equilibrium***,** Workshop on "Nonequilibrium Phenomena, Spin Glasses, and Algorithms", Beijing Satellite Meeting of STATPHYS 25, Kavli Institute for Theoretical Physics China (KITPC), Beijing, China, July 1-5, 2013.

157. *Wirbel, Wellen Energie: alles ist Physik,* Vorlesung bei der KinderUni 2013, Universität Wien, 10. Juli 2013.

158. *Zwischen Ordnung und Chaos: Zufall und Unverhersagbarkeit in der Physik,* Carinthische Dialoge, St. Urban, Austria, July 26-28, 2013.

159. *Computational statistical mechanics: Rare events in complex systems,* 5 lectures at the „Summer School on Statistical Physics of Complex and Small Systems", Instituto de Fisica Interdisciplinar y Sistemas Complejos (IFISC), Palma de Mallorca, Spain, September 2-12, 2013.

160. *Studying nucleation processes with computer simulations: Neural networks for force calculations and structure recognition,* CECAM/Psi-k Research Conference „Multiscale Modelling from First Principles 2013, Platja d'Aro, Spain", September 8-13, 2013.

161. *From freezing to friction: Defects in the dynamics of colloidal monolayers in equilibrium and non-equilibrium states,* Seminar at the Department of Chemistry, Universidad Complutense, Madrid, Spain, October 25, 2013.

162. *Computational Physics: das virtuelle Labor im Supercomputer*, Öffentlicher Vortrag im Rahmen der *Physik Matinee 2013*, Fakultät für Physik, Universität Wien, 7. Dezember 2013.

163. *Irreversibility at an non-equilibrium fluctuations at the nanoscale: Dynamics relaxation of a levitated nanoparticle*, Conference „Five computational pieces and a do: celebrating the 70th birthday of Giovanni Ciccotti", Universitá di Roma „La Sapienza, Roma, Italy", December 18-20, 2013.

164. *From freezing to friction: Defects in the dynamics of colloidal monolayers in equilibrium and non-equilibrium states*, Seminar at the Department of Physics, Lyon, France, January 17, 2014.

165. *Parallel software suite for neural network potentials for materials simulations*, 4th VSC User Meeting, Neusiedl am See, Austria, February 24, 2014.

166. *Cavitation in water at negative pressure*, CECAM-Workshop „Long time dynamics from short trajectories", Lugano, Switzerland, March 12, 2014.

167. *Studying nucleation processes with computer simulations: from freezing to cavitation*, *ESF*-Workshop „Atmospheric ice nucleation", Vienna, Austria, April 26, 2014.

168. *Computational Physics: das virtuelle Labor im Supercomputer*, Bundesrealgymnasium Wien 14, Linzerstraße 146, May 7, 2014.

169. *Making holes in water: Cavitation in water at negative pressure*, Workshop „WATER 2014, Metastability and nucleation in Water: theory, experiments and applications", Les Houches, France, June 1-6, 2014.

169. *A Neural Network Based Potential for Water*, Gordon Conference „Water and aqueous solutions", Holdenerss, New Hampshire, USA, July 27-August 1, 2014.

170. *Cavitation in water at negative pressure*, EMLG-JMLG Annual Conference „Molecular Liquids and Soft Matter: from Fundamentals to Applications", Rome, Italy, 8-12 September, 2014.

171. *Irreversibilität: von der Boltzmanngleichung zu den Fluktuationstheoremen*, 64. Jahrestagung der Österreichischen Physikalischen Gesellschaft, Boltzmanntagung, Pöllau, Austria, 26 September 2014.

172. *Making holes in water: cavitation under tension*, Statistical Mechanics in Physics, Chemistry and Biology: A symposium celebrating David Chandler's 70th birthday, MIT, Cambridge, MA, USA, 18-19 October, 2014.

173. *Irreversibility and non-equilibrium fluctuations of a levitated nanoparticle*, Workshop on Recent Developments in Non-Equilibrium Physics, „Luxemburg out of Equilibrium", University of Luxemburg, Luxemburg, 12-15 January, 2015.

174. *Simulating nucleation and growth processes: From cavitation to crystallization,* Free Energy Workshop 2015, Münster, Germany, 8-10 March, 2015.

175. *Bridging time, length and energy scales in simulations of condensed matter,* Austrian HPC Meeting 2015, Obergurgl, Austria, 15-20 March, 2015.

176. *Irreversibiity and the meaning of the Second Law at the Nanoscale,* KFU-TU Physics Colloquium, Technical University of Graz, Graz, Austria, 28 April, 2015.

177. *Irreversibiity and the Second Law at the nanoscale: fluctuation theorem for relaxation of a levitated particle from a non-equilibrium steady state,* Theoretical-Physical Chemistry Colloquium, Technical University of Munich, Munich, Germany, 4 May, 2015.

178. *Irreversibiity and non-equilibrium fluctuations of a levitated nano particle,* Mainz Materials Simulation Days 2015 – Non-equilibrium processes in soft matter, Max Planck Institute for Polymer Research, Mainz, Germany, 10-12 June, 2015.

179. *Pathways to self-assembly: crystallization by nucleation and growth* (four lectures), Enrico Fermi Summer School on „Soft Matter Self-Assembly*",* Villa Monastero, Varenna, Italy, June 29-July 7, 2015.

180. *Wirbel, Wellen Energie: alles ist Physik,* Vorlesung bei der KinderUni 2015, Universität Wien, 7. Juli 2015.

181. *Cavitation in water under tension,* Gordon Research Conference on the „Chemistry and Physics of Liquids", Holderness School, Holderness, NH, USA, August 2-7, 2015.

182. *Cavitation in water under tension,* Group Retreat 2015, Plonerhof, Rodeneck, Südtirol, September 3-6, 2015.

183. *Non-equilibrium methods for equilibrium free energy computations,* Bad Honnef Physics School on „Entropy and Information: the statistical mechanics perspective", Physikzentrum Bad Honnef, Bad Honnef, Germany, 13-18 September 2015.

184. *A neural network potential for water: Effect of van der Waals interactions on the thermodynamics, structure and dynamics of water,* FISMAT 2015 - Italian National Conference on Condensed Matter Physics, Palermo, Italy, 28 September – 2 October 2015.

185. *How van-der-Waal's interactions determine the unique properties of water: insights from neural network based simulations,* Workshop on Water at the Interface between Biology, Chemistry, Physics and Materials Sciences , ICTP, Trieste, Italy, 5-9 October 2015.

186. *Towards a common format for molecular mechanis simulations,* Workshop „Towards a Common Format for Computational Materials Science Data", CECAM. Lausanne, Switzerland, 25-27 January 2016.

187. *How van-der-Waal's interactions determine the unique properties of water: insights from neural network based simulations,* Workshop „Physics of biomolecules: structure, dynamics, and function", Brixen, Italy, 3-6 February 2016.

188. *How van-der-Waal's interactions determine the unique properties of water: insights from neural network based simulations,* Soiree of the Thomas-Young-Center, London, UK, 10 March 2016.

189. *Four Lectures on „Statistical Sampling Methods: Monte Carlo and Molecular Dynamics Simulations",* HPC-LEAP School "Numerical Analysis and Algorithms at the Exascale: Classical N-body Methods for Complex Systems on Massively Parallel Architectures", Forschungszentrum Jülich, Jülich, Germany, 7-8 April 2016.

190. *Simulating water and ice using neural network potentials,* 115th Statistical Mechanics Conference, Rutgers University, New Brunswick, NJ, USA, 8-10 May 2016.

191. *Non-equilibrium Methods for Equilibrium Free Energy Computations,* Summer School „Classical and Quantum Non-equilibrium Dynamics“, The Raymond and Berverly Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv, Israel, 3-5 August 2016.

192. *Irreversibility and Non-equilibrium Fluctuations at the Nanoscale: Dynamic Relaxation of a Levitated Glass Bead,* Workshop „Classical and Quantum Non-equilibrium Dynamics“, The Raymond and Berverly Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv, Israel, 7-10 August 2016.

193. *Reaction coordinate for freezing: do we understand crystallization?,* CECAM-Lorentz Workshop „Reaction coordinates from molecular simulations“, Lorentz Center, Leiden, The Netherlands, 29 August-2 September 2016.

194. *Exploring the Free Energetics and Kinetics of Nucleation Processes: from Crystallization to Cavitation,* Summer School on „Exploring and quantifying rough free energy landscapes“, Ettore Majorana Foundation and Center for Scientific Culture, Erice, Italy, 7-12 October 2016.

195. *Simulating rare events in complex molecular systems: from transition state theory to basic transition path sampling*, ECAM Extended Software Development Workshop on „Trajectory Sampling“*,* Internationale Akademie Traunkirchen, Traunkrichen, Austria, 16-25 November 2016.

196. *Statistical Mechanics with one and many particles*, Workshop on “Levitated Nanomechanics”, Capellades, Spain, 26-28 March 2017.

197. *Exploring the free energetics and kinetics of nucleation processes: from crystallization to cavitation,* Seminar at the Dept. of Mechanical and Aerospace Engineering, Sapienza University of Rome, Rome, Itay, 11 May 2017.

198. *How van-der-Waal's interactions determine the unique properties of water: insights from neural network based simulations,* invited keynote talk, 10th Liquid Matter Conference, Ljubljana, Slovenia, 17-12 July 2017.

199. *Scientific challenges: state of the art rare event sampling, basic and advanced path based sampling,* E-CAM Extended Software Development Workshop on Classical Molecular Dynamics, Lorentz Center, Leiden, The Netherlands, 14-25 August 2017.

200. *Machine learning in atomistic simulations: from reaction pathways to phase diagrams,* Symposium on Theoretical Chemistry (STC), “Big Data in Chemistry”, invited keynote lecture, University of Basel, Basel, Switzerland, August 21-25 2017.

201. *Exploring the mechanism and kinetics of nucleation processes: from crystallization to cavitation,* WATOC 2017 (11th Triennial Congress of the World Association of Theoretical and Computational Chemists), invited talk, Munich, Germany, 27 August-1 September 2017.

202. *How van-der-Waal's interactions determine the unique properties of water: insights from neural network based simulations,* invited talk, Joint Meeting of the European and Japanese Molecular Liquids Group EMLG/JMLG, Vienna, Austria, 10-14 September 2017.

203. *Simulating water and ice with neural network potentials,* invited talk, Recent Advances in Modelling Rare Events (RARE2017) Agra, India, 7-10 December 2017.

204. *Bubble nucleation and the stability limit of water under tension,* invited talk, CECAM Workshop "Physics and Chemistry at Fluid/Fluid Interfaces", Erwin Schrödinger Institute, Vienna, Austria, 11-13 December 2017.

Vienna, January 2018