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Tristan Bureau

Employment	Heidelberg University, Institute for Theoretical Physics Professor (W3)	2023–
	IMC Trading B.V. Quant	2021–2023
	University of Amsterdam, Van 't Hoff Institute for Molecular Sciences, Informatics Institute Assistant Professor	2020–2021
	Max Planck Institute for Polymer Research, Theory Group Emmy Noether group leader	2016–2019
	Group leader	2014–2016
	University of Basel and Novartis Postdoc	2012–2013
Education	Carnegie Mellon University, Department of Physics Ph.D.	2011
	École Polytechnique Fédérale de Lausanne BSc. Physics	2006
Secondary appointments	Member, IWR Heidelberg.	2023–
	Member, SIMPLAIX.	2023–
	Editorial Board member, Computational Science and Engineering, Springer Nature.	2023–
	Committee member, Diversity & Inclusion, HIMS, UvA.	2021
	Committee member, National Agenda for Computational Sciences, NWO.	2021
	Data-driven discovery and design	
	HIMS PhD Lectures, UvA.	2020–2021
	Guest Editor, APL Materials Special Issue.	2020
	“Discovering Patterns in Disorder: Machine Learning for Fluctuating Mesoscopic Materials,” together with Dr. Alpha Lee and Prof. Daan Frenkel (U. Cambridge)	
	Editorial Board member, Machine Learning: Science and Technology, IOP Publishing.	2019–
	Steering-committee member, Carl-Zeiss-Stiftung on Algorithmic Intelligence.	2019–2020


Board member, TRR146.	2018–2020
Deputy member representative, FAIR-DI e.V. (FAIR Data Infrastructure). Pillar C: Soft-matter and biomolecular simulations	2018–
Deputy member representative, Max Planck Network BiGmax. Project Area 4: Learning thermodynamic properties of materials	2017–
Co-Head, TRR146 Integrated research training group (IRTG).	2017–2020
Junior PI, Max Planck Graduate Center (graduate school MPIP/JGU Mainz).	2017–2020
Awards “Hochschullehrer-Nachwuchs-Workshop 2019,” Marl, Germany.	2019
Invitation by GDCh Makromolekulare Chemie to selected young university lecturers	
“Machine Learning for Physics and the Physics of Learning,” CA USA.	09–12/2019
Invited core participant of IPAM Long Program	
Examination authorization (Prüfungsberechtigung), Physics, JGU Mainz.	2018
Emmy Noether Program, Deutsche Forschungsgemeinschaft (DFG). Independent research group, Equivalence to Habilitation	2016
Astrid and Bruce McWilliams Fellowship, CMU, Pittsburgh, PA USA. 1-year full tuition and stipend scholarship	2010
Student Travel Award – Biophysical Society Meeting, San Francisco, CA.	2010
Guy C. Berry Graduate Research Award – Mellon College of Science, CMU.	2009
Funding FAIRmat: consortium of the German Research-Data Infrastructure NFDI. Area C2: Multiscale modeling	2022–
Roche Postdoctoral Fellow: Machine Learning for Crystal Structure Prediction. With F. Hoffmann-La Roche AG, Avant-garde Materials Simulation GmbH Role: Co-supervisor	2021–2022
Simulating catalysis: Multiscale embedding of machine learning potentials. EPSRC (UK) grant Role: Project partner	2021–2022
Carl-Zeiss-Stiftung “Algorithmic Intelligence as Emergent Phenomenon”. One of 4 core co-PIs (Consortium: €3.0M) Statistical predictability of physical systems (€0.2M)	2019–2023
Max Planck Network BiGmax on “Big Data in Materials Science”. Automated analysis of atom force probe detector maps (€0.2M) Learning thermodynamic properties of materials (€0.2M)	2018–2022
Emmy Noether Program, Deutsche Forschungsgemeinschaft (DFG). Independent research group (€1.3M) Topic: Importance Sampling in Chemical Space	2016–2020
TRR146 “Multiscale Modeling in Soft Matter”. A6: Dynamics in multiscale simulations (€0.2M)	2014–2022

B7: Machine learning in multiscale simulations (€0.2M)

Academic interviews	Theoretical Physics in soft condensed matter. University of Heidelberg. W3 professor position. Offer, accepted	05/2022
	Machine learning in the physical sciences. University of Stuttgart. W3 professor position	06/2021
	Department of Physics. University of Stuttgart. W3 professor position	11/2020
	Computational Soft Matter. University of Amsterdam. Tenure-track assistant professor position. Offer, accepted	03/2019
	Theory of Condensed Matter Physics. University of Konstanz. Tenure-track professor position	11/2018
	Data science in the natural sciences. SISSA, Trieste. Tenure-track professor position	02/2018
	Computational materials modeling. SEAS, Harvard University. Tenure-track assistant professor position	04/2017
Teaching (courses)	Computational statistics and data analysis. Heidelberg University.	Fall 2023
	Generative learning for molecular systems. Heidelberg University.	Fall 2023
	Introduction Computational Science. University of Amsterdam. Co-taught with Dr. Valeria Krzhizhanovskaya	Spring 2021
	Statistical Thermodynamics of Complex Molecular Systems. University of Amsterdam. Co-taught with Prof. Peter Bolhuis, Dr. Bernd Ensing	Fall 2020
	Advanced computer simulation techniques. JGU Mainz. Co-taught with Dr. Giovanni Settanni, Dr. Omar Valsson	Spring 2019
	Computer simulation techniques. JGU Mainz. Co-taught with Dr. Giovanni Settanni, Dr. Peter Virnau	Fall 2018
	Polymer physics and soft-matter theory. JGU Mainz. Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji	Fall 2018
	Advanced computer simulation techniques. JGU Mainz. Co-taught with Dr. Denis Andrienko, Dr. Giovanni Settanni	Spring 2018
	Polymer physics and soft-matter theory. JGU Mainz. Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji	Fall 2017
	Polymer physics and soft-matter theory. JGU Mainz. Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji	Fall 2016
	Advanced computer simulation techniques. JGU Mainz. Co-taught with Dr. Denis Andrienko, Dr. Giovanni Settanni	Spring 2016
	Electronic structure calculations. University of Basel.	Fall 2012

Co-taught with Prof. Markus Meuwly

Teaching (guest lectures)	Machine learning for physics and astronomy. UvA/Vu (Amsterdam).	10/2020
	Machine learning for coarse-grained simulations	
	Biomolecular simulations. UvA (Amsterdam).	05/2020
	Machine learning for coarse-grained simulations	
Teaching (summer schools)	MolSim 2020. UvA (Amsterdam).	01/2020
	CECAM: “Applied mathematics and machine learning perspectives on Big Data”. Mainz.	10/2019
	CECAM/TRR School on Machine Learning. Mainz.	09/2018
	CCCS School on machine learning in atomistic simulations. Vallico Sotto, Italy.	05/2017
	CCCS School on coarse-graining. Engelberg, Switzerland.	03/2017
	ESPResSo++/VOTCA tutorial. Schloss Waldthausen, Mainz.	10/2014
Tutoring	CECAM/TRR School on Machine Learning. Mainz.	09/2018
	CCCS School on coarse-graining. Engelberg, Switzerland.	03/2017
	ESPResSo++/VOTCA tutorial. Schloss Waldthausen, Mainz.	10/2014
	ESPResSo workshop. University of Stuttgart.	10/2010
	Workshop “Coarse-Grained Biomolecular Modeling”. Levi, Finland.	03/2010
Workshop organization	CECAM: “(Machine) learning how to coarse-grain”. Online event (Zoom & Discord). 260 registered participants	09/2020
	CECAM: “Applied mathematics and machine learning perspectives on Big Data Problems in Computational Sciences,”. CECAM.	10/2019
	Mainz Materials Simulation Days 2019. Max Planck Institute for Polymer Research.	06/2019
	International workshop for MaxNet on Big Data in Materials Science. Dresden.	04/2019
	CECAM/TRR School on Machine Learning. Mainz. 60 participants	09/2018
	CECAM: “New frontiers in particle-based multiscale modeling”. CECAM.	09/2018
	Mainz Materials Simulation Days 2015. Max Planck Institute for Polymer Research. 100+ participants	06/2015
	ESPResSo++/VOTCA tutorial. Schloss Waldthausen.	10/2014
Invited talks	CECAM workshop: FAIR and TRUE Data in Soft Matter Simulations. Mainz, Germany.	09/2023
	Comp Chem Exchange, Merck KGaA. Darmstadt, Germany.	09/2023
	ELLIS unit Heidelberg. Heidelberg, Germany.	07/2023
	TMCQ2023. Seoul, South Korea.	06/2023
	MMSD 2023: Biology in soft matter. Mainz, Germany.	06/2023

BiGmax School on Artificial Intelligence for Materials Science. Cap Roig, Spain.	05/2023
SIMPLAIX Workshop “ML for Multiscale Molecular Modeling”. Heidelberg, Germany.	05/2023
CECAM Modeling Materials at Realistic time Scales. Berlin, Germany.	07/2022
MMSML Workshop. Barcelona, Spain.	07/2022
Lorentz “Accelerating the Understanding of Rare Events”. Leiden, Netherlands.	09/2021
CECAM “Non-covalent interactions in large molecules”. Lausanne, Switzerland.	08/2021
PASC21 Conference. Geneva, Switzerland.	07/2021
CECAM “Local structure meets machine learning in soft matter systems”. Switzerland.	06/2021
Dutch Soft Matter meeting. virtual.	05/2021
SIAM Conference “Mathematical Aspects of Materials Science”. virtual.	05/2021
GDCh Bunsen-Tagung 2021. virtual.	05/2021
Plenary speaker	
Department of Physics, University of Delaware. Newark, USA (virtual).	03/2021
Minisymposium of the SFB CRC 1114. Berlin, Germany (virtual).	03/2021
Minisymposium of the SFB TRR 102. Halle, Germany (virtual).	02/2021
Institute for Materials Science, TU Dresden. Dresden, Germany (virtual).	12/2020
Department of Chemistry, Boston University. Boston, USA (virtual).	10/2020
CECAM Multiscale simulations of soft matter. virtual.	09/2020
AI4Science Colloquium Series. University of Amsterdam, Amsterdam (virtual).	06/2020
CECAM “Open Databases Integration for Materials Design”. virtual.	06/2020
Conference on A FAIR Data Infrastructure for Materials Genomics. virtual.	06/2020
 online recording	
CompBioMed “Machine learning meets modelling and simulation methods”. virtual.	03/2020
online recording	
PComS Seminar Series. Tohoku University, Sendai, Japan.	02/2020
Department of Chemical Engineering, Kyoto University. Kyoto, Japan.	02/2020
CANES Seminar Series. King’s College London, London, United Kingdom.	02/2020
Physics@Veldhoven. Veldhoven, Netherlands.	01/2020
University of Marburg. Marburg, Germany.	11/2019
E-CAM “Building a molecular foundry”. virtual.	11/2019
Leibniz Institute for Interactive Materials. Aachen, Germany.	11/2019
IPAM “Machine Learning for Physics and the Physics of Learning”. UCLA, USA.	10/2019
online recording	
CECAM “Beyond machine learning for quantum chemistry”. Bremen, Germany.	10/2019
“Hochschullehrer-Nachwuchs-Workshop 2019”. Marl, Germany.	09/2019
IPAM “Machine Learning for Physics and the Physics of Learning”. UCLA, USA.	09/2019
online recording	

American Chemical Society (ACS) Fall Meeting 2019 . San Diego, CA USA.	08/2019
XXXI IUPAP Conference on Computational Physics (CCP2019) . Hong Kong.	07/2019
Advances in methods for multi-scale modelling,. Leiden, Netherlands.	06/2019
“MolKin2019 Sampling, Design and Machine Learning” . Berlin, Germany.	06/2019
IPAM “Many-Particle Systems with Machine Learning” . Lake Arrowhead, USA.	06/2019
German Physical Society (DPG) meeting . Regensburg.	03/2019
American Physical Society (APS) meeting . Boston, USA.	03/2019
Machine Learning and Reverse engineering for Soft Materials. Leiden, Netherlands.	12/2018
Integrating Molecular Simulation with Machine Learning. Leiden, Netherlands.	10/2018
Max Planck Institute for Iron Research. Düsseldorf, Germany.	08/2018
Modern Approaches to Coupling Scales In Materials Simulations. Lenggries, Germany.	07/2018
Many-Particle Systems with Machine Learning . Lake Arrowhead, USA.	06/2018
Computational Chemistry Days . Helsinki, Finland.	05/2018
Keynote lecture	
Theoretical Computational Chemistry Workshop. Engelberg, Switzerland.	05/2018
SimTech Conference . Stuttgart, Germany.	03/2018
German Physical Society (DPG) meeting . Berlin, Germany.	03/2018
Cross-sectional symposium	
Department of Applied Mathematics. TU Eindhoven, Eindhoven, The Netherlands.	02/2018
Department of Chemistry. Ruhr University of Bochum, Bochum, Germany.	01/2018
German Chemical Society (GDCh) Satellite Meeting. Berlin, Germany.	09/2017
Symposium on Theoretical Chemistry (STC) . University of Basel.	08/2017
Department of Physical Chemistry. University of Münster.	07/2017
Department of Physical Chemistry. University of Göttingen.	06/2017
IPAM “Many-Particle Systems with Machine Learning” . UCLA, USA.	11/2016
Department of Chemistry. Free University of Brussels.	04/2016
Department of Chemistry. University of Konstanz.	04/2016
“Transferability Issues in Multiscale Modelings” . Mainz.	12/2015
Department of Chemistry. Freie Universität Berlin.	11/2015
CCCS Symposium on Machine Learning. Basel, Switzerland.	11/2015
Statistical Physics and Low Dimensional Systems. Pont-à-Mousson, France.	05/2015
“Modeling Many-Body Interactions 2015” . Lake Garda, Italy.	05/2015
CSP Workshop . University of Georgia, Athens GA USA.	03/2015
Faculty of Natural Sciences. University of Groningen.	06/2015
Mainz Materials Simulations Day (MMSD 2013). Mainz, Germany.	06/2013
Department of Chemistry. Penn State.	05/2013
Laboratoire de Biochimie Théorique. CNRS, Paris VII, France.	01/2013







	Forschungszentrum Jülich. Jülich, Germany.	11/2012
	Max Planck Institute for Polymer Research. Mainz.	07/2010
	INSERM. Paris, France.	06/2010
	Max Planck Institute for Polymer Research. Mainz.	07/2009
	Forschungszentrum Jülich. Jülich.	07/2009
Supervision	Diego van der Mast. Bachelor student.	2021
	Menno Bruin. Bachelor student.	2020
	Bernadette Mohr. Ph.D. student.	2019–2023
	Atreyee Banerjee. Postdoc.	2019–2022
	Yasemin Bozkurt Varolgüneş. Exchange Ph.D. student.	2018–2019
	Martin Girard. Postdoc.	2018–2021
	Humboldt fellowship	
	René Scheid. Master student.	2018–2019
	Timon Wittenstein. Bachelor student.	2018–2019
	Clemens Rauer. Postdoc.	2018–2019
	Arghya Dutta. Postdoc.	2018–2021
	Marc Stieffenhofer. Ph.D. student.	2018–2022
	MPGC fellowship	
	Christian Hoffmann. Diplom student.	2018–2019
	Bernadette Mohr. Diplom student.	2018–2019
	Alessia Centi. Postdoc.	2017–2019
	Kiran H. Kanekal. Ph.D. student.	2016–2020
	MPGC fellowship. Graduated with Summa Cum Laude (highest distinction)	
	Roberto Menichetti. Postdoc.	2016–2018
	Svenja Wörner. Ph.D. student.	2016–2020
	Marius Bause. Ph.D. student.	2016–2020
	MAINZ fellowship	
	Joseph F. Rudzinski. Postdoc.	2015–2019
	Humboldt fellowship	
	Chan Liu. Ph.D. student.	2014–2019
Doctoral defense committees	Manuel Carrer. University of Oslo.	09/2023
	Elham Kianiharchegani. Western University.	08/2023
	Marc Stieffenhofer. Max Planck Institute for Polymer Research.	06/2022
	Marius Bause. University of Amsterdam.	01/2021














Kiran H. Kanekal. Max Planck Institute for Polymer Research.	12/2020
Yasemin Bozkurt Varolgüneş. Koç University.	05/2020
Chan Liu. Max Planck Institute for Polymer Research.	10/2019

Journal referee

ACS Central Science, ACS Macro Letters, ACS Omega, Accounts of Chemical Research, Advanced Theory and Simulations, Advances in Physics: X, Biochimica et Biophysica Acta (BBA) - Biomembranes, Biointerphases, Biophysical Journal, Chemical Physics, Chemical Science, ChemistryOpen, Computer Physics Communications, EPL (Europhysics Letters), Interface Focus, Journal of Applied Physics, Journal of Chemical Information and Modeling, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Journal of Computational Physics, Journal of Computational Science, Journal of Membrane Biology, Journal of Molecular Modeling, Journal of Physical Chemistry Letters, Langmuir, Machine Learning: Science and Technology, Molecular Systems Design & Engineering, Nature Communications, New Journal of Physics, Physical Chemistry Chemical Physics, Physical Review Letters, Plos One, Polymer Crystallization, SciPost Physics, Science Advances, Scientific Reports, Soft Matter, The Journal of Chemical Physics, The Journal of Physical Chemistry














Publications










74. Luca M. Ghiringhelli, Carsten Baldauf, Tristan Bereau, Sandor Brockhauser, Christian Carbogno, Javad Chamanara, Stefano Cozzini, Stefano Curtarolo, Claudia Draxl, Shyam Dwaraknath, Adam Fekete, James Kermode, Christoph T. Koch, Markus Kühbach, Alvin Noe Ladines, Patrick Lambrix, Maja-Olivia Himmer, Sergey V. Levchenko, Micael Oliveira, Adam Michalchuk, Ronald E. Miller, Berk Onat, Pasquale Pavone, Giovanni Pizzi, Benjamin Regler, Gian-Marco Rignanese, Jörg Schaarschmidt, Markus Scheidgen, Astrid Schneidewind, Tatyana Sheveleva, Chuanxun Su, Denis Usvyat, Omar Valsson, Christof Wöll, Matthias Scheffler. Shared metadata for data-centric materials science. *Sci Data* 10 (2023) 
73. Bernadette Mohr, Diego Van Der Mast, Tristan Bereau. Condensed-Phase Molecular Representation to Link Structure and Thermodynamics in Molecular Dynamics. *J. Chem. Theory Comput.* (2023) 
72. Kübra Kaygisiz, Arghya Dutta, Lena Rauch-Wirth, Christopher Synatschke, Jan L. Münch, Tristan Bereau, Tanja Weil. Inverse design of viral infectivity-enhancing peptide fibrils from continuous protein-vector embeddings. *Biomater. Sci.* (2023) 
71. Arghya Dutta, Tristan Bereau, Thomas A. Vilgis. Identifying Sequential Residue Patterns in Bitter and Umami Peptides. *ACS Food Sci. Technol.* 2 (2022) 
70. Kiran Kanekal, Joseph Rudzinski, Tristan Bereau. Broad chemical transferability in structure-based coarse-graining. *J. Chem. Phys.* 157 (2022) 
69. Marc Stieffenhofer, Christoph Scherer, Falk May, Tristan Bereau, Denis Andrienko. Benchmarking coarse-grained models of organic semiconductors via deep backmapping. *Front. Chem.* 10 (2022) 















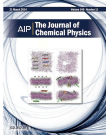

68. Matthias Scheffler, Martin Aeschlimann, Martin Albrecht, Tristan Bereau, Hans-Joachim Bungartz, Claudia Felser, Mark Greiner, Axel Groß-Klußmann, Christoph T. Koch, Kurt Kremer, Wolfgang E. Nagel, Markus Scheidgen, Christof Wöll, Claudia Draxl. FAIR data enabling new horizons for materials research. *Nature* 604 (2022)  
67. Isabel Kleinwächter, Bernadette Mohr, Aljoscha Joppe, Nadja Hellmann, Tristan Bereau, Heinz D. Osiewacz, Dirk Schneider. CLiB – a novel cardiolipin-binder isolated via data-driven and in vitro screening. *RSC Chem. Biol.* 3 (2022)  
Special Issue: Biological Membranes as Targets to Natural and Synthetic Compounds
66. Bernadette Mohr, Kirill Shmilovich, Isabel Kleinwächter, Dirk Schneider, Andrew Ferguson, Tristan Bereau. Data-driven discovery of cardiolipin-selective small molecules by computational active learning. *Chem. Sci.* 13 (2022)  
65. Martin Girard, Tristan Bereau. Induced asymmetries in membranes. *Biophysical Journal* 122 (2022)
64. Padmabati Mondal, Pierre-André Cazade, Akshaya Kumar Das, Tristan Bereau, Markus Meuwly. Multipolar Force Fields for Amide-I Spectroscopy from Conformational Dynamics of the Alanine Trimer. *J. Phys. Chem. B* 125 (2021)  
63. Arghya Dutta, Jilles Vreeken, Luca M. Ghiringhelli, Tristan Bereau. Publisher’s Note: “Data-driven equation for drug–membrane permeability across drugs and membranes” [*J. Chem. Phys.* 154, 244114 (2021)]. *The Journal of Chemical Physics* 155 (2021)
62. Arghya Dutta, Jilles Vreeken, Luca M. Ghiringhelli, Tristan Bereau. Data-driven equation for drug–membrane permeability across drugs and membranes. *The Journal of Chemical Physics* 154 (2021)  
61. Joseph Rudzinski, Sebastian Kloth, Svenja Wörner, Tamisra Pal, Kurt Kremer, Tristan Bereau, Michael Vogel. Dynamical properties across different coarse-grained models for ionic liquids. *J. Phys.: Condens. Matter* 33 (2021)  
60. Martin Girard, Tristan Bereau. Computer simulations of lipid regulation by molecular semigrand canonical ensembles. *Biophysical Journal* 120 (2021)  
59. Martin Girard, Tristan Bereau. Finite-size transitions in complex membranes. *Biophysical Journal* 120 (2021)  
58. Marius Bause, Tristan Bereau. Reweighting non-equilibrium steady-state dynamics along collective variables. *J. Chem. Phys.* 154 (2021)  
57. Isabel Kleinwächter, Stefanie Pannwitt, Alessia Centi, Nadja Hellmann, Eckhard Thines, Tristan Bereau, Dirk Schneider. The Bacteriostatic Activity of 2-Phenylethanol Derivatives Correlates with

- Membrane Binding Affinity. *Membranes* 11 (2021)  
56. Marc Stieffenhofer, Tristan Bereau, Michael Wand. Adversarial reverse mapping of condensed-phase molecular structures: Chemical transferability. *APL Materials* 9 (2021)  
 Guest editor for Special Issue: “Discovering Patterns in Disorder: Machine Learning for Fluctuating Mesoscopic Materials”
 55. Tristan Bereau. Computational compound screening of biomolecules and soft materials by molecular simulations. *Modelling Simul. Mater. Sci. Eng.* 29 (2020)  
 Invited Topical Review
 54. Joseph Rudzinski, Tristan Bereau. Coarse-grained conformational surface hopping: Methodology and transferability. *The Journal of Chemical Physics* 153 (2020)  
 Editor’s Pick
 53. Marc Stieffenhofer, Michael Wand, Tristan Bereau. Adversarial reverse mapping of equilibrated condensed-phase molecular structures. *Mach. Learn.: Sci. Technol.* 1 (2020)  
 52. Martin Girard, Tristan Bereau. Regulating Lipid Composition Rationalizes Acyl Tail Saturation Homeostasis in Ectotherms. *Biophysical Journal* 119 (2020)  
 Featured in T. R. Shaw, S. L. Veatch, New and Notable: The Membrane “Pull” That Balances Metabolism’s “Push” in Lipid Homeostasis, *Biophys. J.* 119 (2020)
 Featured in CMU Biophysics Blog: “It takes a membrane to raise a lipid”
 51. Clemens Rauer, Tristan Bereau. Hydration free energies from kernel-based machine learning: Compound-database bias. *The Journal of Chemical Physics* 153 (2020)  
 Invited contribution to Special Issue “Machine Learning Meets Chemical Physics”
 50. J. Wesley Barnett, Connor Bilchak, Yiwen Wang, Brian Benicewicz, Laura A. Murdock, Tristan Bereau, Sanat K. Kumar. Designing exceptional gas-separation polymer membranes using machine learning. *Sci. Adv.* 6 (2020)  
 Press releases on EurekaAlert!
 Press releases on Phys.org
 49. Christoph Scherer, René Scheid, Denis Andrienko, Tristan Bereau. Kernel-Based Machine Learning for Efficient Simulations of Molecular Liquids. *J. Chem. Theory Comput.* 16 (2020)  
 LAMMPS custom implementation
 VOTCA repository
 48. Yasemin Bozkurt Varolgunes, Tristan Bereau, Joseph Rudzinski. Interpretable embeddings from molecular simulations using Gaussian mixture variational autoencoders. *Mach. Learn.: Sci. Technol.* 1 (2020)  







47. Alessia Centi, Arghya Dutta, Sapun Parekh, Tristan Bereau. Inserting Small Molecules across Membrane Mixtures: Insight from the Potential of Mean Force. *Biophysical Journal* 118 (2020) 
46. Christian Hoffmann, Alessia Centi, Roberto Menichetti, Tristan Bereau. Molecular dynamics trajectories for 630 coarse-grained drug-membrane permeations. *Sci Data* 7 (2020) 
 [figshare database of 15,120 molecular dynamics trajectories](#)
45. Amelie Koch, Svenja Morsbach, Tristan Bereau, Gaëtan Lévêque, Hans-Jürgen Butt, Markus Deserno, Katharina Landfester, George Fytas. Probing Nanoparticle/Membrane Interactions by Combining Amphiphilic Diblock Copolymer Assembly and Plasmonics. *J. Phys. Chem. B* 124 (2020) 
 Cover article 
44. Chan Liu, Jan Gerit Brandenburg, Omar Valsson, Kurt Kremer, Tristan Bereau. Free-energy landscape of polymer-crystal polymorphism. *Soft Matter* 16 (2020) 
[Invited contribution to Special Issue “2021 Soft Matter Emerging Investigators”](#)
43. Svenja Wörner, Tristan Bereau, Kurt Kremer, Joseph Rudzinski. Direct route to reproducing pair distribution functions with coarse-grained models via transformed atomistic cross correlations. *J. Chem. Phys.* 151 (2019) 
42. Marius Bause, Timon Wittenstein, Kurt Kremer, Tristan Bereau. Microscopic reweighting for nonequilibrium steady-state dynamics. *Phys. Rev. E* 100 (2019) 
41. Kiran Kanekal, Tristan Bereau. Resolution limit of data-driven coarse-grained models spanning chemical space. *J. Chem. Phys.* 151 (2019) 
40. Roberto Menichetti, Tristan Bereau. Revisiting the Meyer-Overton rule for drug-membrane permeabilities. *Molecular Physics* 117 (2019) 
 Invited contribution to Special Issue Liblice 2018
39. Christian Hoffmann, Roberto Menichetti, Kiran Kanekal, Tristan Bereau. Controlled exploration of chemical space by machine learning of coarse-grained representations. *Phys. Rev. E* 100 (2019) 
 [Zenodo database of 1.3M drug-membrane transfer free energies](#)
38. Martin Girard, Ali Ehlen, Anisha Shakya, Tristan Bereau, Monica Olvera De La Cruz. Hoobas: A highly object-oriented builder for molecular dynamics. *Computational Materials Science* 167 (2019) 
37. Corinna Schilling, Thomas Mack, Selene Lickfett, Stefanie Sieste, Francesco S. Ruggeri, Tomas Sneideris, Arghya Dutta, Tristan Bereau, Ramin Naraghi, Daniela Sinske, Tuomas Knowles, Christopher Synatschke, Tanja Weil, Bernd Knöll. Sequence-Optimized Peptide Nanofibers as Growth Stimulators for Regeneration of Peripheral Neurons. *Adv. Funct. Mater.* 29 (2019) 

36. Roberto Menichetti, Kiran Kanekal, Tristan Bereau. Drug–Membrane Permeability across Chemical Space. *ACS Cent. Sci.* 5 (2019) 
 [Database of 500k permeability coefficients](#)
35. Joseph Rudzinski, Marc Radu, Tristan Bereau. Automated detection of many-particle solvation states for accurate characterizations of diffusion kinetics. *The Journal of Chemical Physics* 150 (2019) 
34. Svenja Morsbach, Grazia Gonella, Volker Mailänder, Seraphine Wegner, Si Wu, Tobias Weidner, Rüdiger Berger, Kaloian Koynov, Doris Vollmer, Noemí Encinas, Seah Ling Kuan, Tristan Bereau, Kurt Kremer, Tanja Weil, Mischa Bonn, Hans-Jürgen Butt, Katharina Landfester. Engineering Proteins at Interfaces: From Complementary Characterization to Material Surfaces with Designed Functions. *Angew. Chem. Int. Ed.* 57 (2018) 
33. Chan Liu, Kurt Kremer, Tristan Bereau. Polymorphism of Syndiotactic Polystyrene Crystals from Multiscale Simulations. *Adv. Theory Simul.* 1 (2018) 
32. Tristan Bereau, Robert Distasio, Alexandre Tkatchenko, Anatole Von Lilienfeld. Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning. *The Journal of Chemical Physics* 148 (2018) 
 Invited contribution to Special Issue Data-Enabled Theoretical Chemistry
 Selected as Featured Article by the Editorial Board
 [Press release on AIP SciLight](#)
 [Original implementation](#)
31. Joseph Rudzinski, Tristan Bereau. Structural-kinetic-thermodynamic relationships identified from physics-based molecular simulation models. *The Journal of Chemical Physics* 148 (2018) 
30. Roberto Menichetti, Kurt Kremer, Tristan Bereau. Efficient potential of mean force calculation from multiscale simulations: Solute insertion in a lipid membrane. *Biochemical and Biophysical Research Communications* 498 (2017) 
 Invited contribution to Special Issue Multiscale Modeling
29. Joseph Rudzinski, Tristan Bereau. The Role of Conformational Entropy in the Determination of Structural-Kinetic Relationships for Helix-Coil Transitions. *Computation* 6 (2018) 
28. Tristan Bereau, Joseph Rudzinski. Accurate Structure-Based Coarse Graining Leads to Consistent Barrier-Crossing Dynamics. *Phys. Rev. Lett.* 121 (2018) 
 [ESPResSo++ implementation](#)
27. Roberto Menichetti, Kiran Kanekal, Kurt Kremer, Tristan Bereau. In silico screening of drug-membrane thermodynamics reveals linear relations between bulk partitioning and the potential of mean

- force. *The Journal of Chemical Physics* 147 (2017) 
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