Heidelberg University
Institute for Theoretical Physics
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Tristan Bereau

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). 2018–
Pillar C: Soft-matter and biomolecular simulations

Deputy member representative, Max Planck Network BiGmax. 2017–
Project Area 4: Learning thermodynamic properties of materials

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). 2016
Independent research group, Equivalence to Habilitation

Astrid and Bruce McWilliams Fellowship, CMU, Pittsburgh, PA USA. 2010
1-year full tuition and stipend scholarship

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. 2022–
Area C2: Multiscale modeling

Roche Postdoctoral Fellow: Machine Learning for Crystal Structure Prediction. 2021–2022
With F. Hoffmann-La Roche AG, Avant-garde Materials Simulation GmbH
Role: Co-supervisor

Simulating catalysis: Multiscale embedding of machine learning potentials. 2021–2022
EPSRC (UK) grant
Role: Project partner

Carl-Zeiss-Stiftung "Algorithmic Intelligence as Emergent Phenomenon". 2019–2023
One of 4 core co-PIs (Consortium: €3.0M)
Statistical predictability of physical systems (€0.2M)

Max Planck Network BiGmax on "Big Data in Materials Science". 2018–2022
Automated analysis of atom force probe detector maps (€0.2M)
Learning thermodynamic properties of materials (€0.2M)

Emmy Noether Program, Deutsche Forschungsgemeinschaft (DFG). 2016–2020
Independent research group (€1.3M)
Topic: Importance Sampling in Chemical Space

TRR146 "Multiscale Modeling in Soft Matter". 2014–2022
A6: Dynamics in multiscale simulations (€0.2M)

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

Academic interviews

Theoretical Physics in soft condensed matter. University of Heidelberg. 05/2022
W3 professor position. Offer, accepted

Machine learning in the physical sciences. University of Stuttgart. 06/2021
W3 professor position

Department of Physics. University of Stuttgart. 11/2020
W3 professor position

Computational Soft Matter. University of Amsterdam. 03/2019
Tenure-track assistant professor position. Offer, accepted

Theory of Condensed Matter Physics. University of Konstanz. 11/2018
Tenure-track professor position

Data science in the natural sciences. SISSA, Trieste. 02/2018
Tenure-track professor position

Computational materials modeling. SEAS, Harvard University. 04/2017
Tenure-track assistant professor position

Teaching (courses)

MVComp2 Computational statistics and data analysis. Heidelberg University. Summer 2024
Co-taught with Prof. Daniel Durstewitz

MVSpec Soft matter physics. Heidelberg University. Summer 2024
Co-taught with Dr. Falko Ziebert

MVSpec Machine learning in the biomolecular world. Heidelberg University. Summer 2024
Co-taught with Prof. Rebecca Wade

MVComp2 Computational statistics and data analysis. Heidelberg University. Fall 2023

Generative learning for molecular systems. Heidelberg University. Fall 2023

Introduction Computational Science. University of Amsterdam. Spring 2021
Co-taught with Dr. Valeria Krzhizhanovskaya

Statistical Thermodynamics of Complex Molecular Systems. University of Amsterdam. Fall 2020
Co-taught with Prof. Peter Bolhuis, Dr. Bernd Ensing

Advanced computer simulation techniques. JGU Mainz. Spring 2019
Co-taught with Dr. Giovanni Settanni, Dr. Omar Valsson

Computer simulation techniques. JGU Mainz. Fall 2018
Co-taught with Dr. Giovanni Settanni, Dr. Peter Virnau

Polymer physics and soft-matter theory. JGU Mainz. Fall 2018
Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji

Advanced computer simulation techniques. JGU Mainz. Spring 2018
Co-taught with Dr. Denis Andrienko, Dr. Giovanni Settanni

Polymer physics and soft-matter theory. JGU Mainz. Fall 2017

Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji

Polymer physics and soft-matter theory. JGU Mainz. Fall 2016
Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji

Advanced computer simulation techniques. JGU Mainz. Spring 2016
Co-taught with Dr. Denis Andrienko, Dr. Giovanni Settanni

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

CCSC2024: Chemical Compound Space Conference 2024. Heidelberg Conference Center. 05/2024

CECAM: "(Machine) learning how to coarse-grain". Online event (Zoom & Discord). 09/2020
260 registered participants

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. 09/2018
60 participants

CECAM: "New frontiers in particle-based multiscale modeling". CECAM. 09/2018

Mainz Materials Simulation Days 2015. Max Planck Institute for Polymer Research. 06/2015
100+ participants

ESPResSo++/VOTCA tutorial. Schloss Waldthausen. 10/2014

Invited talks

ECT* Workshop Bridging Scales". Trento, Italy. 04/2024
Institute for Computational Physics, University of Stuttgart. Stuttgart, Germany. 04/2024
DWI - Leibniz Institute for Interactive Materials. Aachen, Germany. 03/2024
CCRC1114 Colloquium. Berlin, Germany. 02/2024
Institute of Physics, Freiburg University. Freiburg, Germany. 02/2024
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

Bálint Maté. Visiting Ph.D. student. 2024
Daniel Nagel. Postdoc. 2023–
Luis Walter. Ph.D. student. 2023–
Osman Oezdemir. Master student. 2023–2024
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. MPGC fellowship. Graduated with Summa Cum Laude (highest distinction)	2016–2020
Roberto Menichetti. Postdoc.	2016–2018
Svenja Wörner. Ph.D. student.	2016–2020
Marius Bause. Ph.D. student. MAINZ fellowship	2016–2020
Joseph F. Rudzinski. Postdoc. Humboldt fellowship	2015–2019
Chan Liu. Ph.D. student.	2014–2019

Doctoral defense committees

Robert Chojowski. Heidelberg University.	01/2024
Bernadette Mohr. University of Amsterdam.	12/2023
Onur Caylak. TU Eindhoven.	12/2023
Benedikt Rennekamp. Heidelberg University.	10/2023
Johannes Blumberg. Heidelberg University.	10/2023
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

75. Luca M. Ghiringhelli, Carsten Baldauf, Tristan Bereau, Sandor Brockhauser, Christian Carbogno, Javad Chamanara, Stefano Cozzini, Stefano Curtarolo, Claudia Draxl, Shyam Dwaraknath, Ádám 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)

74. Kübra Kaygisiz, Lena Rauch-Wirth, Arghya Dutta, Xiaoqing Yu, Yuki Nagata, Tristan Bereau, Jan L. Münch, Christopher Synatschke, Tanja Weil. Data-mining unveils structure–property–activity correlation of viral infectivity enhancing self-assembling peptides. Nat Commun 14 (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. Martin Girard, Tristan Bereau. Induced asymmetries in membranes. Biophysical Journal 122 (2022)

70. Arghya Dutta, Tristan Bereau, Thomas A. Vilgis. Identifying Sequential Residue Patterns in Bitter and Umami Peptides. ACS Food Sci. Technol. 2 (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. Kiran Kanekal, Joseph Rudzinski, Tristan Bereau. Broad chemical transferability in structure-based coarse-graining. J. Chem. Phys. 157 (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. 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)

65. 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)

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. Martin Girard, Tristan Bereau. Finite-size transitions in complex membranes. Biophysical Journal 120 (2021)

60. Martin Girard, Tristan Bereau. Computer simulations of lipid regulation by molecular semigrand canonical ensembles. Biophysical Journal 120 (2021)

59. Marius Bause, Tristan Bereau. Reweighting non-equilibrium steady-state dynamics along collective variables. J. Chem. Phys. 154 (2021)

58. 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)

57. 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"

56. 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)

55. Joseph Rudzinski, Tristan Bereau. Coarse-grained conformational surface hopping: Methodology and transferability. The Journal of Chemical Physics 153 (2020)

    Editor's Pick

54. Tristan Bereau. Computational compound screening of biomolecules and soft materials by molecular simulations. Modelling Simul. Mater. Sci. Eng. 29 (2020)

Invited Topical Review

53. Marc Stieffenhofer, Michael Wand, Tristan Bereau. Adversarial reverse mapping of equilibrated condensed-phase molecular structures. Mach. Learn.: Sci. Technol. 1 (2020)

52. 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"

51. 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"

50. 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"

49. 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 EurekAlert!

    Press releases on Phys.org

48. 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

47. Yasemin Bozkurt Varolgunes, Tristan Bereau, Joseph Rudzinski. Interpretable embeddings from molecular simulations using Gaussian mixture variational autoencoders. Mach. Learn.: Sci. Technol. 1 (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. 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)

44. 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

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. 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

39. 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)

38. 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)

37. Roberto Menichetti, Tristan Bereau. Revisiting the Meyer-Overton rule for drug-membrane permeabilities. Molecular Physics 117 (2019)

Invited contribution to Special Issue Liblice 2018

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. Tristan Bereau, Joseph Rudzinski. Accurate Structure-Based Coarse Graining Leads to Consistent Barrier-Crossing Dynamics. Phys. Rev. Lett. 121 (2018)

ESPResSo++ implementation

33. Joseph Rudzinski, Tristan Bereau. Structural-kinetic-thermodynamic relationships identified from physics-based molecular simulation models. The Journal of Chemical Physics 148 (2018)

32. Chan Liu, Kurt Kremer, Tristan Bereau. Polymorphism of Syndiotactic Polystyrene Crystals from Multiscale Simulations. Adv. Theory Simul. 1 (2018)

31. 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)

30. 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

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. 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)

27. 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)

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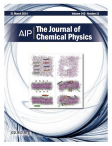

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Dissemination

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