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

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)

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

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

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

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

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* (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)]. *J. Chem. Phys.* 155 (2021)

62. Arghya Dutta, Jilles Vreeken, Luca M. Ghiringhelli, Tristan Bereau. Data-driven equation for drug–membrane permeability across drugs and membranes. *J. Chem. Phys.* 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. *J. Chem. Phys.* 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. *J. Chem. Phys.* 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 EurekAlert!

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. *J. Chem. Phys.* 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)

26. Johannes Franz, Tristan Bereau, Stefanie Pannwitt, Veerappan Anbazhagan, Alexander Lehr, Udo Nubbemeyer, Ulrich Dietz, Mischa Bonn, Tobias Weidner, Dirk Schneider. Nitrated Fatty Acids Modulate the Physical Properties of Model Membranes and the Structure of Transmembrane Proteins. *Chem. Eur. J.* 23 (2017)

25. Qiran Xiao, Yanping Chen, Tristan Bereau, Yunfeng Shi. An in-silico walker. *Chemical Physics Letters* 659 (2016)

24. Joseph Rudzinski, Tristan Bereau. Concurrent parametrization against static and kinetic information leads to more robust coarse-grained force fields. *Eur. Phys. J. Spec. Top.* 225 (2016)

    Invited contribution to Special Issue "Modern Simulation Approaches in Soft Matter Science: From Fundamental Understanding to Industrial Applications"

23. Krystel El Hage, Tristan Bereau, Sofie Jakobsen, Markus Meuwly. Impact of Quadrupolar Electrostatics on Atoms Adjacent to the Sigma-Hole in Condensed-Phase Simulations. *J. Chem. Theory Comput.* 12 (2016)

22. Tristan Bereau, Denis Andrienko, Kurt Kremer. Research Update: Computational materials discovery in soft matter. *APL Mater.* 4 (2016)

    Invited contribution to Special Issue The Materials Genome Initiative

21. Tristan Bereau, Kurt Kremer. Protein-Backbone Thermodynamics across the Membrane Interface. *J. Phys. Chem. B* 120 (2016)

    Invited contribution to Special Issue William M. Gelbart Festschrift

20. Joseph Rudzinski, Kurt Kremer, Tristan Bereau. Communication: Consistent interpretation of molecular simulation kinetics using Markov state models biased with external information. *The Journal of Chemical Physics* 144 (2016)

    Invited contribution to Special Issue Markov Models of Molecular Kinetics

19. Tristan Bereau, W. F. Drew Bennett, Jim Pfaendtner, Markus Deserno, Mikko Karttunen. Folding and insertion thermodynamics of the transmembrane WALP peptide. *The Journal of Chemical Physics* 143 (2015)

    Invited contribution to Special Issue "Coarse graining of macromolecules, biopolymers, and membranes"

18. Tristan Bereau. Better Together: Lipopeptide Micelle Formation Enhances Antimicrobial Selectivity. *Biophysical Journal* 109 (2015)

    Invited contribution by Editors for "New and Notable"

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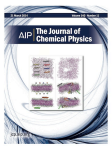

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