

Heidelberg University
Institute for Theoretical Physics
Philosophenweg 19
69120 Heidelberg, Germany

+49-6221-54-9448 📞
bureau@uni-heidelberg.de @
@tristanbureau 🐦
https://tristanbureau.com 🌐
0000-0001-9945-1271 🆔

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 Group leader	2016–2019 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	Spokesperson, Artificial Intelligence (AI) Board, Heidelberg University.	2024–
	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. Data-driven discovery and design	2021
	HIMS PhD Lectures, UvA.	2020–2021
	Guest Editor, APL Materials Special Issue. “Discovering Patterns in Disorder: Machine Learning for Fluctuating Mesoscopic Materials,” together with Dr. Alpha Lee and Prof. Daan Frenkel (U. Cambridge)	2020
	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).	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 PhD project, Deutsche Forschungsgemeinschaft (DFG).	2025–2028
Generative machine learning in the grand canonical ensemble (€0.2M)	
Field of Focus 2 of Heidelberg University.	2024
FAIRmat: consortium of the German Research-Data Infrastructure NFDI.	2022–
Area C2: Multiscale modeling	
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.	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). 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) B7: Machine learning in multiscale simulations (€0.2M)	2014–2022
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)	MVBP2 Theoretical Biophysics. Heidelberg University.	Summer 2025
	MVSpec Soft matter physics. Heidelberg University. Co-taught with Dr. Falko Ziebert	Summer 2025
	MKTP1 Theoretical statistical physics. Heidelberg University.	Winter 2024
	MVComp2 Computational statistics and data analysis. Heidelberg University. Co-taught with Prof. Daniel Durstewitz	Summer 2024
	MVSpec Soft matter physics. Heidelberg University. Co-taught with Dr. Falko Ziebert	Summer 2024
	MVSpec Machine learning in the biomolecular world. Heidelberg University. Co-taught with Prof. Rebecca Wade	Summer 2024
	MVComp2 Computational statistics and data analysis. Heidelberg University.	Winter 2023
	Generative learning for molecular systems. Heidelberg University.	Winter 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	<i>Spring 2019</i>
	Computer simulation techniques. JGU Mainz. Co-taught with Dr. Giovanni Settanni, Dr. Peter Virnau	<i>Fall 2018</i>
	Polymer physics and soft-matter theory. JGU Mainz. Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji	<i>Fall 2018</i>
	Advanced computer simulation techniques. JGU Mainz. Co-taught with Dr. Denis Andrienko, Dr. Giovanni Settanni	<i>Spring 2018</i>
	Polymer physics and soft-matter theory. JGU Mainz. Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji	<i>Fall 2017</i>
	Polymer physics and soft-matter theory. JGU Mainz. Co-taught with Prof. Burkhard Dünweg, Dr. Sara Jabbari-Farouji	<i>Fall 2016</i>
	Advanced computer simulation techniques. JGU Mainz. Co-taught with Dr. Denis Andrienko, Dr. Giovanni Settanni	<i>Spring 2016</i>
	Electronic structure calculations. University of Basel. Co-taught with Prof. Markus Meuwly	<i>Fall 2012</i>
Teaching (guest lectures)	Machine learning for physics and astronomy. UvA/Vu (Amsterdam).	<i>10/2020</i>
	Machine learning for coarse-grained simulations	
	Biomolecular simulations. UvA (Amsterdam).	<i>05/2020</i>
	Machine learning for coarse-grained simulations	
Teaching (summer schools)	MolSim 2020. UvA (Amsterdam).	<i>01/2020</i>
	CECAM: “Applied mathematics and machine learning perspectives on Big Data”. Mainz.	<i>10/2019</i>
	CECAM/TRR School on Machine Learning. Mainz.	<i>09/2018</i>
	CCCS School on machine learning in atomistic simulations. Vallico Sotto, Italy.	<i>05/2017</i>
	CCCS School on coarse-graining. Engelberg, Switzerland.	<i>03/2017</i>
	ESPResSo++/VOTCA tutorial. Schloss Waldthausen, Mainz.	<i>10/2014</i>
Tutoring	CECAM/TRR School on Machine Learning. Mainz.	<i>09/2018</i>
	CCCS School on coarse-graining. Engelberg, Switzerland.	<i>03/2017</i>
	ESPResSo++/VOTCA tutorial. Schloss Waldthausen, Mainz.	<i>10/2014</i>
	ESPResSo workshop. University of Stuttgart.	<i>10/2010</i>
	Workshop “Coarse-Grained Biomolecular Modeling”. Levi, Finland.	<i>03/2010</i>
Workshop organization	2025 ESPResSo Summer School. Stuttgart, Germany.	<i>10/2025</i>
	3rd SIMPLAIX Workshop on Machine Learning for Multiscale Molecular Modeling. Heidelberg, Germany.	<i>05/2025</i>

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 [Chalmers AI4Science Seminar](#). Gothenburg, Sweden. 02/2025
 [online recording](#)

TCP Workshop. Luxembourg, Luxembourg.	12/2024
IWR Colloquium . Heidelberg, Germany.	11/2024
Workshop: Physics of Intelligence and Machine Learning 2024 . Heidelberg, Germany.	10/2024
Workshop: Machine-Learning-Based Sampling in Lattice Field Theory and Quantum Chemistry . Bonn, Germany.	10/2024
CECAM Flagship School: Simulating soft matter across scales. Stuttgart, Germany.	10/2024
Multiscale Simulations of Soft Matter IV . Darmstadt, Germany.	09/2024
CECAM Workshop: Bridging the Atomic-Mesoscale Gap for Complex Interfaces . Montpellier, France.	09/2024
CECAM Workshop: Leveraging Machine Learning for Sampling Rare Events in Biomolecular Systems . Mainz, Germany.	09/2024
31st CMD-General Conference of the Condensed Matter Division of the European Physical Society . Braga, Portugal.	08/2024
IDA-BIFOLD-ML Group retreat. Berlin, Germany.	08/2024
Physics department, Heidelberg University. Heidelberg, Germany.	06/2024
Institute of Physical Chemistry, Karlsruhe Institute of Technology. Karlsruhe, Germany.	05/2024
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	Gerrit Gerhartz. PhD student.	2025–
	Sander Hummerich. PhD student.	2025–
	co-supervised with Prof. Ullrich Köthe, IWR Heidelberg	
	Daniel Hofmann. Master student.	2025–
	Magnus Schümann. Bachelor student.	2025
	Selina Pohl. Master student.	2024–
	Luis Vazquez-Salazar. Postdoc.	2024–
	SNSF postdoc fellowship	
	Aleksander Durumeric. Postdoc.	2024–2025
	FI EMS interdisciplinary postdoc fellowship	
	Leticia Gómez. Postdoc.	2024–2025
	co-supervised with Dr. Christopher Synatschke, MPIP Mainz	
	Dominic Holst. Master student.	2024–
	Bálint Maté. Visiting Ph.D. student.	2024
	SNSF fellowship	
	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.	2016–2020
MPGC fellowship . Graduated with <i>Summa Cum Laude</i> (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	Haoxiang Zhao. TU Eindhoven.	03/2025
	Lennart Rover. Heidelberg University.	01/2025
	Roman Remme. Heidelberg University.	01/2025
	Simon L. Krug. Technische Universität Berlin.	12/2024
	Oliver Drozdowski. Heidelberg University.	11/2024
	Gianmarco Camazzola. Heidelberg University.	10/2024
	Manuel Brenner. Heidelberg University.	07/2024
	Dominik Lemm. University of Vienna.	03/2024
	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** 80. Tristan Bereau, Luis J. Walter, Joseph Rudzinski. Martignac: Computational Workflows for Reproducible, Traceable, and Composable Coarse-Grained Martini Simulations. *J. Chem. Inf. Model.* **64** (2024)  
-  [Streamlit app](#)
-  [Github repository](#)
-  [Online talk](#)
79. Bálint Máté, François Fleuret, Tristan Bereau. Neural Thermodynamic Integration: Free Energies from Energy-Based Diffusion Models. *J. Phys. Chem. Lett.* **15** (2024)  
-  [Github repository](#)
-  [Online talk](#)
78. Andrea Anelli, Hanno Dietrich, Philipp Ectors, Frank Stowasser, Tristan Bereau, Marcus Neumann, Joost Van Den Ende. Robust and efficient reranking in crystal structure prediction: a data driven method for real-life molecules. *CrystEngComm* **26** (2024) 
77. Ganna Gryn'Ova, Tristan Bereau, Carolin Müller, Pascal Friederich, Rebecca C. Wade, Ariane Nunes-Alves, Thereza A. Soares, Kenneth M. Merz, Jr.. EDITORIAL: Chemical Compound Space Exploration by Multiscale High-Throughput Screening and Machine Learning. *J. Chem. Inf. Model.* **64** (2024)  
76. Stefan Bauer, Peter Benner, Tristan Bereau, Volker Blum, Mario Boley, Christian Carbogno, C Richard A Catlow, Gerhard Dehm, Sebastian Eibl, Ralph Ernstorfer, Ádám Fekete, Lucas Foppa, Peter Fratzl, Christoph Freysoldt, Baptiste Gault, Luca M Ghiringhelli, Sajal K Giri, Anton Gladyshev, Pawan Goyal, Jason Hattrick-Simpers, Lara Kabalan, Petr Karpov, Mohammad S Khorrami, Christoph T.

Koch, Sebastian Kokott, Thomas Kosch, Igor Kowalec, Kurt Kremer, Andreas Leitherer, Yue Li, Christian Liebscher, Andrew Logsdail, Zhongwei Lu, Felix Luong, Andreas Marek, Florian Merz, Jaber R. Mianroodi, Jörg Neugebauer, Zongrui Pei, Thomas A R Purcell, Dierk Raabe, Markus Rampp, Mariana Rossi, Jan-Michael Rost, James Saal, Ulf Saalmann, Kasturi Narasimha Sasidhar, Alaukik Saxena, Luigi Sbailò, Markus Scheidgen, Marcel Schloz, Daniel F Schmidt, Simon Raphael Teshuva, Annette Trunschke, Ye Wei, Gerhard Weikum, Rui Patrick Xian, Yi Yao, Junqi Yin, Meng Zhao, Matthias Scheffler. Roadmap on data-centric materials science. *Modelling Simul. Mater. Sci. Eng.* **32** (2024)



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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)
 Press release on Phys.org
 Press release on (idw) Informationsdienst Wissenschaft
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.* **19** (2023)
 Github repository
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.* **11** (2023)
 Gitlab repository
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)
 Github repository

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. *The Journal of Chemical Physics* **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)  
-  [Blogpost on Pharma's Almanac](#)
-  [Article on Analytik News](#)
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)  
-  [Featured in M. Aldeghi, C. W. Coley, A focus on simulation and machine learning as complementary tools for chemical space navigation, *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) 
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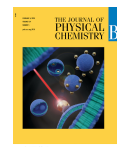
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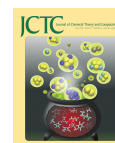
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