Prof. Dr. Barbara Kirchner

Personal Data

Title	Prof. Dr.
First name	Barbara
Name	Kirchner
Current position	Full Professor (W3)
Current institution(s)/site(s), country	Mulliken Center for Theoretical Chemistry, Clausius-Institute of Physical and Theoretical Chemistry, Rheinische Friedrich-Wilhelms-University Bonn, Beringstraße 4, 53115 Bonn, Germany
Identifiers/ORCID	orcid.org/0000-0001-8843-7132

Qualifications and Career

Stages	Periods and Details
Degree programme	Diploma in Chemistry, 1996, TU Chemnitz, Germany
Doctorate	12/1995–06/1999 Mentor: H. Huber, PhD in Theoretical Chemistry, University of Basel, Switzerland
Stages of academic/professional career	Since 2013 Full Professor (W3), Mulliken Center for Theoretical Chemistry, Clausius-Institute of Physical and Theoretical Chemistry, University of Bonn, Germany 2007 – 2012 Full Professor, Chair of Theoretical Chemistry, University of Leipzig, Germany 2003 – 2006 Postdoc (S. D. Peyerimhoff), Clausius-Institute of Physical and Theoretical Chemistry, University of Bonn, Germany 2001 – 2003 Postdoc (J. Hutter), Institute of Organic Chemistry, University of Zürich, Switzerland 2000 – 2001 Postdoc (D. Marx), Institute of Theoretical Chemistry, University of Bochum, Germany 1999 – 2000 Postdoc (D. Marx, M. Parinello), Max-Planck Institute of Solid State Research, Stuttgart, Germany

Activities in the Research System

Committee involvement & activities in the field of academic self-governance:

Since 2024	Deputy Editor of *The Journal of Physical Chemistry B*
Since 2024	Co-Spokesperson of the CRC 1639 (NuMeriQS)
Since 2020	Commission for Advice on Security Relevant Research with substantial Hazard Potential, University of Bonn
2020 – 2022	Head of the department of chemistry, University of Bonn
2020 – 2022	Structural Commission, Faculty of Mathematics and Natural Sciences, University of Bonn
2019 – 2022	Committee on Scientific Instrumentation and Information Technology, DFG
2016 – 2019	Member of the Commission on IT Infrastructure, DFG
Since 2016	Member of the Editorial board of *Topics in Current Chemistry*

Since 2016	Credit Recognition, Chemistry Department, University of Bonn
Since 2016	Member of Examination board Food Chemistry, University of Bonn
2008 – 2012	Equal opportunity commissioner, Chemistry Department, University of Leipzig

Academic Distinctions: Ruth Lynden-Bell Award, ILMAT V, Paris, France (2019); Invited Professor, University of Strasbourg, France (2019); The Inman Lecture, Molten Salts and Ionic Liquids Discussion Group, Royal Society of Chemistry, UK (2017); Invitation to the European Union's "Chairmen of the European Research Councils' Chemistry Committees", St. Malo, France (2004); Scholar of Novartis Foundation, Swiss National Science Foundation, Max-Planck-Society, German Research Foundation (1998 – 1999).

Scientific Results

Citations: 16400, h-index: 68, i10-index: 211 (Google Scholar, 21.03.2024)

Category A (* corresponding author)

1. J. Blasius, K. Drysch, F.H. Pilz, T. Frömbgen, P. Kielb*, **B. Kirchner*** "Efficient Prediction of Mole Fraction Related Vibrational Frequency Shifts" *J. Phys. Chem. Lett.* **2023**, 14, 10531–10536. DOI: 10.1021/acs.jpclett.3c02761.
2. J. Blasius, **B. Kirchner*** "Selective Chirality Transfer to the Bis(trifluoromethylsulfonyl)imide Anion of an Ionic Liquid" *Chem. Eur. J.* **2023**, 29, e202301239. DOI: 10.1002/chem.202301239.
3. V. Alizadeh, F. Malberg, A.A.H. Pádua*, **B. Kirchner*** "Are There Magic Compositions in Deep Eutectic Solvents? Effects of Composition and Water Content in Choline Chloride/Ethylene Glycol from Ab Initio Molecular Dynamics" *J. Phys. Chem. B* **2020**, 124, 7433–7443. DOI: 10.1021/acs.jpcb.0c04844.
4. J. Blasius, J. Ingenmey, E. Perlt, M. von Domaros, O. Hollóczki, **B. Kirchner*** "Predicting mole-fraction-dependent dissociation for weak acids" *Angew. Chem. Int. Ed.* **2019**, 58, 3212–3216. DOI: 10.1002/anie.201811839.
5. P. Ray, A. Balducci, **B. Kirchner*** "Molecular Dynamics Simulations of Lithium-Doped Ionic-Liquid Electrolytes" *J. Phys. Chem. B* **2018**, 122, 10535–10547. DOI: 10.1021/acs.jpcb.8b06022.
6. J. Ingenmey, S. Gehrke, **B. Kirchner*** "How to harvest Grotthuss diffusion in protic ionic liquid electrolyte systems" *ChemSusChem* **2018**, 11, 1900–1910. DOI: 10.1002/cssc.201800436.
7. S. Gehrke, M. von Domaros, R. Clark, O. Hollóczki, M. Brehm, T. Welton, A. Luzar, **B. Kirchner*** "Structure and lifetimes in ionic liquids and their mixtures" *Faraday Discuss.* **2018**, 206, 219–245. DOI: 10.1039/C7FD00166E.
8. R. Macchieraldo, L. Esser, R. Elfgen, P. Voepel, S. Zahn, B.M. Smarsly, **B. Kirchner*** "Hydrophilic Ionic Liquid Mixtures of Weakly and Strongly Coordinating Anions with and without Water" *ACS Omega* **2018**, 3, 8567–8582. DOI: 10.1021/acsomega.8b00995.
9. M. Thomas, M. Brehm, R. Fligg, P. Vöhringer, **B. Kirchner*** "Computing vibrational spectra from *ab initio* molecular dynamics" *Phys. Chem. Chem. Phys.* **2013**, 15, 6608–6622. DOI: 10.1039/C3CP44302G.

10. M. Brehm, **B. Kirchner*** “TRAVIS - A Free Analyzer and Visualizer for Monte Carlo and Molecular Dynamics Trajectories” *J. Chem. Inf. Model.* **2011**, 51, 2007–2023. DOI: 10.1021/ci200217w.

Category B

Publications

1. J. Ingenmey, O. Hollóczki, **B. Kirchner*** “Ion Pairing in Ionic Liquids” in *Encyclopedia of Ionic Liquids* (Ed.: S. Zhang) **2021**, 1–14. DOI: 10.1007/978-981-10-6739-6_63-1.
2. Ionic Liquids II, in: *Topics in Current Chemistry Collections* (Eds.: **B. Kirchner**, E. Perlt) **2018**. DOI: 10.1007/978-3-319-89794-3.
3. Electronic Effects in Organic Chemistry, in: *Topics in Current Chemistry* (Ed.: **B. Kirchner**) **2014**, 351. DOI: 10.1007/978-3-662-43582-3.
4. Multiscale Molecular Methods in Applied Chemistry, in: *Topics in Current Chemistry* (Eds.: **B. Kirchner**, J. Vrabec) **2012**, 307. DOI: 10.1007/978-3-642-24968-6.
5. Ionic Liquids, in: *Topics in Current Chemistry* (Ed: **B. Kirchner**) **2010**, 290. DOI: 10.1007/978-3-642-01780-3.
6. **B. Kirchner*** “Theory of complicated liquids: Investigation of liquids, solvents and solvent effects with modern theoretical methods” *Phys. Rep.* **2007**, 440, 1–111; Invited Review. DOI: 10.1016/j.physrep.2006.11.005.
7. Klartext: “How good is the networking between science and industry? An interview with Prof. Andreas Gansäuer and Prof. Barbara Kirchner” in *ChemCologne Compact* (01/2022). https://www.chemcologne.de/fileadmin/user_upload/CCC/Dokumente/ChemCologne_Compact_1-2022_01.pdf.

Software

1. TRAVIS – Trajectory Analyzer and Visualizer. Travis is a free tool for analyzing and visualizing trajectories from all kinds of Molecular Dynamics or Monte Carlo simulations: https://www.chemie.uni-bonn.de/kirchner/de/software/travis.
2. Peacemaker – The Quantum Cluster Equilibrium Approach to Liquid Phase Properties. https://www.chemie.uni-bonn.de/kirchner/de/software/peacemaker.
3. CONAN – A Novel Tool to Create and Analyze Liquids in Confined Space. https://www.chemie.uni-bonn.de/kirchner/de/software/conan.