Dr. Michael Schauperl

Date of birth: 25.01.1987
Address: Institute of General, Inorganic and Theoretical Chemistry
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Main Research Interests

- Parameterization of force field charge models
- Hydration enthalpy / entropy in biomolecular recognition
- Polarizable force fields
- Ice binding proteins

Professional Experience

2018 - now **Postdoctoral Researcher**, Universty of California, San Diego, USA (unitl 11/2019) University of Innsbruck, Austria and Charite Berlin, Germany (since 12/2019)

Project lead Erwin Schrödinger fellowship *An Efficient, Polarizable Charge Model for Molecular Simulations;* development of software tools for force field parameterization; member of the Open Force Field Initiative

2017 - 2018 **Postdoctoral Researcher**, Leopold-Franzens University of Innsbruck, Austria

Hydrophobicity studies of small organic molecules, proteases and antibodies; supervision of Bachelor and Master research projects

2013 - 2017 **Research Assistant**, Leopold-Franzens University of Innsbruck, Austria

Organization of laboratory courses, exam preparation and teaching in Theoretical Chemistry; supervision of Bachelor and Master research projects

2011 - 2012 **Tutor**, Leopold-Franzens University of Innsbruck, Austria

Supervision of laboratory courses in Organic and Analytical Chemistry

Education

2013 - 2017 **Doctor in Chemistry (PhD)**, Leopold-Franzens University of Innsbruck, Austria

Thesis work on *Enthalpic and Entropic Contributions to Biomolecular Recognition*; protein and amino acid hydrophobicity and their influence on molecular binding, mechanism of ice binding proteins; cooperation projects with solid-state chemists, physisists

2013 - 2016 **Bachelor of Science in Management and Economics**, Leopold-Franzens University of Innsbruck, Austria

Focus on pharmaceutical site closures and their impact on the stock market

2011 - 2013 **Master of Science in Chemistry**, University College London, UK and Leopold-Franzens University of Innsbruck, Austria

A New Computational Approach to Describe Molecularly Imprinted Polymers

2008 - 2011	**Bachelor of Science in Chemistry**, Leopold-Franzens University of Innsbruck, Austria
	Focus on caltalytic surface reactions
2007 - 2013	**Bachelor of Science in Physics**, Leopold-Franzens University of Innsbruck, Austria
	Low energy electron diffraction of chlorene on palladium

IT Skills

Operating Sys.	Windows, MacOS, Linux
Modeling	MOE, AMBER, PyMOL, VMD, OpenMM, Crystal, VASP, Gaussian, Psi4, ForceBalance, OpenForceField Toolkit
Data Software	Microsoft Office, Origin, Stata, Mathematica
Programming	Python, Bash, C

Languages

German	Native
English	Business fluent (2+ years UK/US residency)

Additional Trainings

04/2017	Agile CreActions – dynamic project management, IAK, Münster, Austria
12/2016	Leading Meetings, Leopold-Franzens University, Innsbruck, Austria
06/2016	Strategic Concepts in Scientific and Industrial Reporting, Leopold-Franzens University, Innsbruck, Austria

Scientific Contributions

Talks	13 oral presentations at scientific meetings / international conferences
Posters	9 poster presentations at scientific meetings / international conferences
Papers	25 publications in peer-reviewed journals

Awards

2018	Karl Schlögl Prize for an outstanding doctoral thesis in chemistry
2017	Erwin Schrödinger Fellowship J4150 by the Austrian Science Fund FWF for his postdoctoral research project (162k EUR funding)
2017	ÖAW Max Kade Fellowship (returned in favour of Schrödinger fellowship)
2017	Science Award 2017 of the Tyrolean Economic Chamber
2017	Dr. Otto Seibert Research Award for an exceptional publication
2017	Conference Travel Grant of the “1669 Research Sponsors’ Association”
2016	Nominated for Dean's List (top 5%) of the Institute of Economics, Leopold-Franzens University of Innsbruck, Austria
2014	Performance Scholarship from the Leopold-Franzens University of Innsbruck, Austria (Bachelor of Science Program in Management and Economics)
2012	Performance Scholarship from the Leopold-Franzens University of Innsbruck, Austria (Master of Science Program in Chemistry)

Publications

25. "Force Field Partial Charges with Restrained Electrostatic Potential version 2." **M. Schauperl**, P. Nerenberg, H. Jang, L. P. Wang, C. I. Bayly, D. L. Mobley, M. K. Gilson, *Communications Chemistry* submitted.

24. "Optimized Mapping of Gas-Phase Quantum Calculations to General Force Field Lennard-Jones Parameters Based on Liquid-State Data." S. Kantonen, H. S. Muddana, N. M. Henriksen, **M. Schauperl**, L. P. Wang, M. K. Gilson, *Journal of Chemical Theory and Computation* submitted.

23. "Benchmarking electronic structure methods for accurate fixed-charge electrostatic models." A. Zhou, **M. Schauperl**, P. Nerenberg, *Journal of Chemical Information and Modeling* submitted.

22. "Performance of DFT functionals for properties of small molecules containing beryllium, tungsten and hydrogen." L. Chen, D. Suess, I. Sukuba, **M. Schauperl**, M. Probst, T. Maihom, A. Mauracher, A. Kaiser, *Journal of Computational Chemistry* submitted.

21. "Hydration of Aromatic Heterocycles as Adversary of π-Stacking." J. Loeffler, **M. Schauperl**, K. R. Liedl, *Journal of Chemical Information and Modeling* 59(10) (2019) 4209-4219.

20. "Coil-Globule Transition Thermodynamics of Poly (N-isopropylacrylamide)." M. Podewitz, Y. Wang, P. K. Quoika, J. Loeffler, **M. Schauperl**, K. R. Liedl, *The Journal of Physical Chemistry B* 123(41) (2019) 8838-8847.

19. "Solvation Free Energy as a Measure of Hydrophobicity: Application to Serine Protease Binding Interfaces." J. Kraml, A. S. Kamenik, F. Waibl, **M. Schauperl**, K. R. Liedl, *Journal of Chemical Theory and Computation* 15(11) (2019) 5872-5882.

18. "Electrostatic Recognition as First Step of Substrate Binding to Serine Proteases." B. J. Waldner, J. Kraml, U. Kahler, A. Spinn, **M. Schauperl**, M. Podewitz, J. E. Fuchs, G. Cruciani, K. R. Liedl, *Journal of Molecular Recognition* 31 (2018) e2727.

17. "$CaB_2S_4O_{16}$ – A borosulfate exhibiting a new structure type with phyllosilicate analogue topology." J. Bruns, M. Podewitz, **M. Schauperl**, K. R. Liedl, H. Huppertz, *Chemistry – A European Journal* 23 (2017) 16773-16781.

16. "Balance between hydration enthalpy and entropy is important for ice binding surfaces in Antifreeze Proteins." **M. Schauperl**, M. Podewitz, T. S. Ortner, F. Waibl, A. Thoeny, T. Loerting, K. R. Liedl, *Scientific Reports* 7 (2017) 11901.

15. "Perspectives on the Future of Ice Nucleation Research: Research Needs and Unanswered Questions Identified from Two International Workshops." I. Coluzza, J. Creamean, M. Rossi, H. Wex, P. Alpert, V. Bianco, Y. Boose, C. Dellago, L. Felgitsch, H. Herrmann, S. Jungblut, Z. Kanji, G. Menzl, B. Moffett, C. Moritz, A. Mutzel, U. Poschl, **M. Schauperl**, J. Scheel, E. Stopelli, F. Stratmann, J. Frohlich, H. Grothe, D. Schmale, *Atmosphere* 8 (2017) 138.

14. "$Ag[B(SO_4)_2]$ – Synthesis, crystal structure, and characterization of the first precious metal borosulfate." J. Bruns, M. Podewitz, **M. Schauperl**, K. R. Liedl, O. Janka, R. Pöttgen, H. Huppertz, *European Journal of Inorganic Chemistry* 34 (2017) 3981-3989.

13. "A Binding Pose Flip Explained via Enthalpic and Entropic Contributions" **M. Schauperl**, P. Czodrowski, J. E. Fuchs, R. G. Huber, B. J. Waldner, M. Podewitz, C. Kramer, K. R. Liedl, *Journal of Chemical Information and Modeling* 2 (2017) 345-354.

12. "High-pressure synthesis and crystal structure of $In_3B_5O_{12}$" D. Vitzthum, **M. Schauperl,** K. R. Liedl, H. Huppertz, *Zeitschrift für Naturforschung B* 72 (2017) 69-76.

11. “Orthorhombic HP-*RE*OF (*RE* = Pr, Nd, Sm-Gd) – High-Pressure Syntheses and Single-Crystal Structures (*RE* = Nd, Sm, Eu)” M. Glätzle, **M. Schauperl,** C. Hejny, M. Tribus, K. R. Liedl, H. Huppertz, *ZAAC - Journal of Inorganic and General Chemistry* 20 (2016) 1134-1142.

10. “Enthalpic and Entropic Contributions to Hydrophobicity” **M. Schauperl**, M. Podewitz, B. J. Waldner, K. R. Liedl, *Journal of Chemical Theory and Computation* 12(9) (2016) 4600-4610.

9. “Protease Inhibitors in View of Peptide Substrate Databases” B. J. Waldner, J. E. Fuchs, **M. Schauperl**, C. Kramer, K. R. Liedl, *Journal of Chemical Information and Modeling* 56 (2016) 1228-1235.

8. “Quantitative Correlation of Conformational Binding Enthalpy with Substrate Specificity of Serine Proteases“ B. J. Waldner, J. E. Fuchs, R. G. Huber, S. v. Grafenstein, **M. Schauperl**, C. Kramer, K. R. Liedl, *Journal of Physical Chemistry B* 120 (2016) 299-308.

7. “New High-Pressure Gallium Borate $Ga_2B_3O_7(OH)$ with Photocatalytic Activity“ D. Vitzthum, **M. Schauperl**, C. M. Strabler, P. Brüggeller, K. R. Liedl, U. J. Griesser, H. Huppertz, *Inorganic Chemistry* 55 (2016) 676-681.

6. “Characterizing Protease Specificity: How Many Substrates Do We Need?“ **M. Schauperl**, J. E. Fuchs, B. J. Waldner, R. G. Huber, C. Kramer, K. R. Liedl, *PLOS One* 10 (2015) e0142658.

5. “Synthesis and characterization of a disordered variant of $KB_5O_7(OH)_2$“ T. S. Ortner, **M. Schauperl**, K. Wurst, T. S. Hofer, H. Huppertz, *Zeitschrift für Naturforschung B* 70 (2015) 649-658.

4. “High-Pressure Synthesis of $Cd(NH_3)_2[B_3O_5(NH_3)]_2$: Pioneering the Way to the Substance Class of Ammine Borates“ G. Sohr, N. Ciaghi, **M. Schauperl**, K. Wurst, K. R. Liedl, H. Huppertz, *Angewandte Chemie International Edition* 54 (2015) 6360-6363.

3. “Structure, Thermal Behavior, and Vibrational Spectroscopy of the Silver Borate AgB_3O_5“ G. Sohr, V. Falkowski, **M. Schauperl**, K. R. Liedl, H. Huppertz, *European Journal of Inorganic Chemistry* (2015) 527-533.

2. “Ice nucleation by water-soluble macromolecules“ B.G. Pummer, C. Budke, S. Augustin-Bauditz, D. Niedermeier, L. Felgitsch, C.J. Kampf, R.G. Huber, K.R. Liedl, T. Loerting, T. Moschen, **M. Schauperl**, M. Tollinger, C.E. Morris, H. Wex, H. Grothe, U. Pöschl, T. Koop, J. Fröhlich-Nowoisky, *Atmospheric Chemistry and Physics* 15 (2015) 4077-4091.

1. “Probing the Structural and Binding Mechanism Heterogeneity of Molecularly Imprinted Polymers” **M. Schauperl**, D. W. Lewis, *Journal of Physical Chemistry B* 119 (2015) 563-571.

Journal Covers

5. “Front Cover: $Ag[B(SO_4)_2]$ – Synthesis, crystal structure, and characterization of the first precious metal borosulfate.“ J. Bruns, M. Podewitz, **M. Schauperl**, K. R. Liedl, O. Janka, R. Pöttgen, H. Huppertz, *European Journal of Inorganic Chemistry* 34 (2017).

4. “Cover Story: Perspectives on the Future of Ice Nucleation Research: Research Needs and Unanswered Questions Identified from Two International Workshops.” I. Coluzza, J. Creamean, M. Rossi, H. Wex, P. Alpert, V. Bianco, Y. Boose, C. Dellago, L. Felgitsch, H. Herrmann, S. Jungblut, Z. Kanji, G. Menzl, B. Moffett, C. Moritz, A. Mutzel, U. Poschl, **M. Schauperl**, J. Scheel, E. Stopelli, F. Stratmann, J. Frohlich, H. Grothe, D. Schmale, *Atmosphere* 8 (2017).

3. “Cover Story: A Binding Pose Flip Explained via Enthalpic and Entropic Contributions” **M. Schauperl**, P. Czodrowski, J. E. Fuchs, R. G. Huber, B. J. Waldner, M. Podewitz, C. Kramer, K. R. Liedl, *Journal of Chemical Information and Modeling* 2 (2017).

2. “Cover Picture: Orthorhombic HP-*RE*OF (*RE* = Pr, Nd, Sm-Gd) – High-Pressure Syntheses and Single-Crystal Structures“ M. Glätzle, **M. Schauperl,** C. Hejny, M. Tribus, K. R. Liedl, H. Huppertz, *ZAAC - Journal of Inorganic and General Chemistry* 20 (2016).

1. “Inside Cover: High-Pressure Synthesis of $Cd(NH_3)_2[B_3O_5(NH_3)]_2$: Pioneering the Way to the Substance Class of Ammine Borates.“ G. Sohr, N. Ciaghi, **M. Schauperl**, K. Wurst, K. R. Liedl, H. Huppertz, *Angewandte Chemie International Edition* 54 (2015).