Jun.-Prof. Dr. Florian Kleemiß

Prizes and Scholarships

- **Bachelor-Teaching-Prize 2024 & 2025**
  Studierendenschaft Chemie RWTH Aachen University
- **PhD Prize of the Swiss Society for crystallography**
  Best PhD-thesis 2020/2021
- **Ed Stevens Award**
  for Excellence in Small Molecule Crystallographic Research 2021
- **Walter Benjamin**
  Own position from the DFG in the Walter-Benjamin-Program
- **PhD-scholarship**
  Studienstiftung des deutschen Volkes
- **PhD-scholarship**
  University of Bremen
- **Student-scholarship**
  Studienstiftung des deutschen Volkes
- **Poster-Prize**
  Cambridge Crystallographic Data Center (Hyderabad 2017)
- **Poster-Prize**
  Organic & Biochemistry - Royal Society of Chemistry (Oviedo 2018)

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Employments

2023 – today — **RWTH Aachen**
Juniorprofessor
Molecular Structure of Condensed Matter with Large Data

2021 – 2023 — **University of Regensburg**
Post-Doc
Method development for the analysis of X-ray diffraction and absorption data

2019 – today — **OlexSys GmbH**
Software-Developer, Regensburg
Olex2, NoSpherA2 und LabSafe

2019 – 2021 — **University of Bern**
PhD-Student
Lab- and Tutorial-assistant, organization of international workshops

2016 – 2019 — **University of Bremen**
Student assistant for lab and IT administrative tasks, AG Grabowsky

Education

University of Bern 2019 – 2020
Doktor phil. nat. Chemistry and Molecular Science, Switzerland
Dissertation: Development of Quantum-Crystallographic Methods for Chemical and Biochemical Applications.
Final grade: summa cum laude

University of Bremen 2016 – 2019
PhD-Project
Scholarship for the project: Sila-Ibuprofen

University of Bremen 2014 – 2016
Master of Science, Chemistry
Title of Master thesis: Crystal and enzyme environmental effects on the electron density of a cysteine protease inhibitor model compound,
Total grade: 1,3

University of Bremen 2011 – 2014
Bachelor of Science, Chemistry
Title of Bachelor thesis: Molecular dynamics simulation of the liquid-solid-interface of different models for argon and water,
Total grade: 1,7

Skills

Languages

German
English
Spanish

Programming

C++
CUDA
Python
LaTeX
HTML
Fortran

System administration

Linux
Windows
Hardware
HPC Cluster construction & maintenance
MS Office

Crystallography/Theory

Quantum-Crystallography
Quantunchemistry
QM/MM
MD

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Research Stays

- Synchrotron Beamtimes, ESRF, Grenoble, France
- Synchrotron Beamtime, APS, Lemont, USA
- Synchrotron Beamtimes, SPring-8, Hyogo, Japan
- Research internship, University of Western Australia, Perth, Australia

Teaching Experience

- Diffraction methods – Master Chemistry
- Modern Methods in Inorganic Chemistry – Bachelor Chemistry
- Computational Chemistry – Bachelor Chemistry
- Inorganic Chemistry III – Coordination-Chemistry – Bachelor Chemistry
- Structure Determination III – SynCat Master
- „From the Crystal to Reflection and Back“– Master Chemistry
- Tutorial and Lab course General Chemistry for Medical Students
- Application of Theoretical Chemistry – Master Chemistry
- Tutorial and Lab course General Chemistry – Bachelor Chemistry
- Tutorial “Math in Natural Science” – Bachelor Chemistry
- Individual Coaching of PhD Student – Bonding Analysis and Crystallography

Participation in Conferences and Meetings

Meeting of the European Crystallographic Association
Poznan, Poland | 2025
Invited talk: „Quantum Crystallographic Refinements from Machine Learning – Performance and Speed Benchmarks“

Erice School for Quantum Crystallography
Erice, Italy | 2025
Organizer of two Workshops:
„NoSpherA2“ and “non-periodic Quantum Chemistry”

BENCh Workshop
Göttingen, Germany | 2025
Invited Talk: “The Feedback Between X-ray Diffraction and Density Functional Theory”

Annual Meeting of the German Association for Crystallography
Hannover, Germany | 2025
Session Chair and Invited Talk: “Accelerating Quantum Crystallographic Refinements Using Effective Core Potentials”

Sagamore Conference of the International Union of Crystallography
New-Delhi, India | 2024
Invited Talk: “AI scattering factors: SALTED-NoSpherA2”

Meeting of the Young Crystallographers
Neu-Isenburg, Germany | 2024
Invited Lecture: “Non-spherical Scattering Factors – A Can of Worms Worth Opening”

Meeting of the European Crystallographic Association
Padova, Italy | 2024
„SALTED-NoSpherA2“
Annual Meeting of the American Crystallographic Society
Denver, USA | 2023
Invited Talk “Systematic Benchmark of Levels of Theory in NoSpherA2-HAR”
Organization Workshop “Olex2 and NoSpherA2”
Annual Meeting of the German Association for Crystallography
Bayreuth, Germany | 2024
Invited Talk: „Systematic Benchmark of Levels of Theory in NoSpherA2-HAR“
IUCr Meeting
Melbourne, Australia | 2023
Resonant elastic scattering treatment by multipolar oscillator model revisited
Annual Meeting of the American Crystallographic Society
Baltimore, USA | 2023
Session Chair “Quantum Crystallography”
Organization Workshop “Olex2 and NoSpherA2”
Réciprocs Workshop for Advanced Crystallography
Aix-en-Provence, France | 2023
NoSpherA2 Workshop
Annual Meeting of the German Association for Crystallography
Frankfurt, Germany | 2023
The treatment of core-electrons in Quantum Crystallography
Annual Meeting of the Swiss Association for Crystallography
Bern, Switzerland | 2022
The treatment of core-electrons in Quantum Crystallography
Meeting of the European Crystallographic Association
Versailles, France | 2022
Poster: „NoSpherA2 from inorganic to protein crystallography“
Talk: „Tackling anomalous X-ray scattering via Waller’s dispersion formula“
International Charge Density Meeting
Aarhus, Denmark | 2022
Invited Talk: „NoSpherA2 - from inorganic to protein crystallography“
Annual Meeting of the German Association for Crystallography
Online | 2022
NoSpherA2 - New possibilities, developments and challenges
Annual Meeting of the Swiss Association for Crystallography
Fribourg, Switzerland | 2021
PhD-Prize Talk
IUCr Meeting
Prag, Czechia | 2021
The benefits and challenges of non-spherical refinements - NoSpherA2
Annual Meeting of the British Crystallographic Association
Online | 2021
Keynote: „NoSpherA2“
Joint Meeting of the Polish and German Crystallographic Associations
Wroclaw, Poland | 2021
Chemical bonding analysis based on routine X-ray diffraction experiments

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Tools for Chemical Bonding
Bremen, Germany | 2019
Local Organizing Committee and IT-Organizer

2nd European Symposium on Chemical Bonds
Oviedo, Spain | 2018
X-ray constrained bonding analysis

Erice School for Quantum Crystallography
Erice, Italy | 2018
Poster: „Quantum crystallography of sila-ibuprofen“
Co-Organizer Workshops: „Hirshfeld Atom Refinement in Olex2“

IUCr Meeting
Hyderabad, India | 2017
Crystal and enzyme environmental effects on the electron density of ibuprofen and sila-ibuprofen

Annual Meeting of the Japanese Crystallographic Association
Mito, Japan | 2016
Crystal and enzyme environmental effects on the electron density of a cysteine protease inhibitor model compound

European Charge Density Meeting
Warsaw, Poland | 2016
Crystal and enzyme environmental effects on the electron density of a cysteine protease inhibitor

Robert F. Stewart School for Electron Density and Related Properties
Nancy, France | 2016
Participant in the XD & MoPro Workshop
Poster: „Crystal and enzyme environmental effects on the electron density of a cysteine protease inhibitor“

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Publications in Peer Reviewed Journals

37) Florian Meurer, Florian Kleemiss, Birgit Hischa, Daniel Brüx, Ann-Cathrin Koch, Michael Bodensteiner, SISYPHOS: An automatic procedure for the serial refinement of single-crystal diffraction data in Olex2, *Struct. Dyn.*, **2025,** *12*, 17, 8554-8564.

36) Florian Meurer, Maximilian Schimpf, Birgit Hischa, Christoph Hennig, Julia Rehbein, Florian Kleemiss, Michael Bodensteiner, Synthesis and quantum crystallographic evaluation of WYLID: YLID's red rival, *J. Appl. Cryst.*, **2025**, *58*, 678-687.

35) Pritam Mahawar, Thayalan Rajeshkumar, Florian Ritter, Thomas P. Spaniol, Ulli Englert, Florian Kleemiss, Laurent Maron, Jun Okuda, Amphoteric Zinc(II) Hydride Cations [ZnH]+: Effect of a Bipyridyl Ligand, *Inorg. Chem.*, **2025,** *64, 17*, 8554-8564.

34) Daniel Brüx, Florian Meurer, Florian Kleemiss, Benchmarking crystal structure refinement: A systematic study on Hirshfeld atom refinement, *Struct. Dyn.*, **2025**, *12(5)*, 054101.

33) Florian Kleemiss, Florian Meurer, Ilya G Shenderovich, M. Bodensteiner, The use of effective core potentials in Hirshfeld atom refinement: making quantum crystallography faster in *NoSpherA2*, *J. Appl. Cryst.*, **2025**, *58*, 374-382.

32) Daniel Brüx, Ben Ebel, Florian Kleemiss, Experimental spin state determination of an iron(II) complex by Hirshfeld atom refinement, *Chem. Eur. J.*, **2025**, e202404017.

31) Andrew C. Boggiano, Chad M. Studvick, Sabyasachi Roy Chowdhury, Julie E. Niklas, Haruko Tateyama, Hongwei Wu, Johannes E. Leisen, Florian Kleemiss, Bess Vlaisavljevich, Ivan A. Popov, Henry S. La Pierre, Praseodynium in the Formal +5 Oxidation State, *Nat. Chem.*, **2025,** *17,* 1005-1010.

30) Ravish Sankollia, Lorraine A. Malaspina, Oleg V. Dolomanov, Peter Luger, Julian J. Holstein, Wolfgang Morgenroth, Florian Kleemiss, Simon Grabowsky, Role of restraints on hydrogen atoms in Hirshfeld Atom Refinement: the case of tri-aspartic acid trihydrate, *Acta Cryst.*, **2025**, *B81*(5), 484-497.

29) Julie Niklas, Kaitlyn Otte, Chad Studvick, Sabyasachi Roy Chowdhury, Bess Vlaisavljevich, John Bacsa, Florian Kleemiss, Ivan Popov, Henry S. La Pierre, A Tetrahedral Neptunium(V) Complex, *Nat. Chem.*, **2024**, *16,* 1490-1495.

28) Florian Kleemiss, Norbert Peyerimhoff, Michael Bodensteiner, Refinement of X-ray and electron diffraction crystal structures using analytical Fourier transforms of Slater-type atomic wavefunctions in *Olex2*, *J. Appl. Cryst.*, **2024**, 57, 161-174.

27) Florian Meurer, Florian Kleemiss, Christoph Riesinger, Gábor Balázs, Vedran Vuković, Ilya G. Shenderovich, Christian Jelsch, Michael Bodensteiner, Probing the Isolobal Relation between Cp'''NiP3 and White Phosphorus by Experimental Charge Density Analysis, *Chem. Eur. J.*, **2024**, e202303762.

26) Emanuel Hupf, Florian Kleemiss, Tobias Borrmann, Rumpa Pal, Joanna M. Krzeszczakowska, Magdalena Woińska, Dylan Jayatilaka, Alessandro Genoni, Simon Grabowsky, The effects of experimentally obtained electron correlation and polarization on electron densities and exchange-correlation potentials, *J. Chem. Phys.*, **2023**, 158, 124103.

25) Hikaru Yanai, Yoshihiko Terajima, Florian Kleemiss, Simon Grabowsky, Takashi Matsumoto, Reversing the Bond Length Alternation Order in Conjugated Polyenes by Susbtituent Effects, *Chem. Eur. J.*, **2023**, 29, e202203538.

24) Kunal Jha, Florian Kleemiss, Michal L. Chodkiewicz, Paulina M Dominiak, Aspherical atom refinements on X-ray data of diverse structures including disordered and covalent organic framework systems: a timeaccuracy trade-off, *J. Appl. Cryst.*, **2023**, 56, 116-127.

23) Florian Meurer, Oleg V. Dolomanov, Christoph Hennig, Norbert Peyerimhoff, Florian Kleemiss, Horst Puschmann, Michael Bodensteiner, Refinement of anomalous dispersion correction parameters in single-crystal structure determinations, *IUCrJ*, **2022**, *9*, 5, 604-609.

22) Sylwia Pawledzio, Maura Malinska, Florian Kleemiss, Simon Grabowsky, Krzysztof Wozniak, Influence of modelling disorder on Hirshfeld atom refinement results of an organo-gold (I) compounds, *IUCrJ*, **2022**, *9*, 4, 497-507.

21) Vanessa F. Schwinghammer, Melissa Janesch, Florian Kleemiss, Stefanie Gärtner, Single Crystal X-Ray Structure Analyses of Binary and Ternary Compounds $A_{49}Tl_{108+x}$ (A=K, Rb, Cs; x=0–1.76) Related to the $K_{49}Tl_{108}$ Type Structure, *ZAAC*, **2022**, e2022001.

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20) Sylwia Pawledzio, Maura Malinska, Florian Kleemiss, Simon Grabowsky, Krzysztof Wozniak, Aurophilic Interactions Studied by Quantum Crystallography, *Inorg. Chem.*, **2022**, *61*, 10,4235-4239.
19) Susanne M. Tiefenthaler, Florian Kleemiss, Nikolaus Korber, [A ([18] crown-6)]$_2$ [Pt (CO)$_3$]·10 NH$_3$ (A= K, Rb) –A crystal structure containing the long postulated [Pt (CO)$_3$]$^{2-}$, *ZAAC*, **2022**, e202100378.
18) Florian Kleemiss, Pim Puylaert, Daniel Duvinage, Malte Fugel, Kunihisa Sugimoto, Jens Beckmann, Simon Grabowsky, Ibuprofen and sila-ibuprofen: polarization effects in the crystal and enzyme environments, *Acta Cryst.*, **2021**, *B77*(6), 892-905.
17) Laura Midgley, Luc J. Bourhis, Oleg V. Dolomanov, Simon Grabowsky, Florian Kleemiss, Horst Puschmann, Norbert Peyerimhoff, Vanishing of the atomic form factor derivatives in non-spherical structural refinement–a key approximation scrutinized in the case of Hirshfeld atom refinement, *Acta Cryst.*, **2021**, *A77*, 519-533.
16) Giulia Novelli, Charles J. McMonagle, Florian Kleemiss, Michael Probert, Horst Puschmann, Simon Grabowsky, Helen E. Maynard-Casely, Garry J. McIntyre, Simon Parsons, Accurate H-atom parameters for the two polymorphs of L-Histidine at 5, 105 and 295 K, *Acta Cryst.*, **2021**, *B77*, 785-800.
15) Sylwia Pawledzio, Maura Malinska, Magdalena Woinska, Jakub Wojciechowski, Lorraine Andrade Malaspina, Florian Kleemiss, Simon Grabowsky, Krzysztof Wozniak, Relativistic Hirshfeld atom refinement of an organo-gold(I) compound, *IUCrJ*, **2021**, *8*, 4, 608-620.
14) Sebastian Holsten, Lorraine A. Malaspina, Florian Kleemiss, Stefan Mebs, Emanuel Hupf, Simon Grabowsky, Jens Bekmann, Different Reactivities of (5-Ph$_2$P-Ace-6-)$_2$MeSiH toward the Rhodium(I) Chlorides [(C$_2$H$_4$)$_2$RhCl]$_2$ and [(CO)$_2$RhCl]$_2$. Hirshfeld Atom Refinement of a Rh–H···Si Interaction, *Organometallics*, **2021**, *40*, 13, 2027-2038.
13) Malte Fugel, Anneke Dittmer, Florian Kleemiss, Simon Grabowsky, On the Role of Hydrogen Bonding in Gas-Phase S$_N$2 Reactions at Silicon, *J. Phys. Chem. A*, **2021**, *125*, 19, 4070-4078.
12) Florian Kleemiss, Horst Puschmann, Oleg V. Dolomanov, Michael Bodensteiner, Norbert Peyerimhoff, Laura Midgley, Luc Bourhis, Alessandro Genoni, Lorraine A. Malaspina, Dylan Jayatilaka, Fraser White, Bernhard Grundkötter, Simon Steinhauer, Dieter Lentz, Simon Grabowsky, Accurate Crystal Structures and Chemical Properties from NoSpherA2, *Chem. Sci.,* **2021**, *12*, 1675-1692.
11) Florian Kleemiss, Erna K. Wieduwilt, Emanuel Hupf, Ming W. Shi, Scott G. Stewart, Dylan Jayatilaka, Michael J. Turner, Kunihisa Sugimoto, Eiji Nishibori, Tanja Schirmeister, Thomas C. Schmidt, Bernd Engels, Simon Grabowsky, Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules, *Chem. Eur. J.,* **2021**, *27*, 3407-3419.
10) Florian Kleemiss, Aileen Justies, Daniel Duvinage, Patrick Watermann, Eric Ehrke, Kunihisa Sugimoto, Malte Fugel, Lorraine A. Malaspina, Anneke Dittmer, Torsten Kleemiss, Pim Puylaert, Nelly R. King, Anne Staubitz, Thomas M. Tzschentke, Ralf Dringen, Simon Grabowsky, Jens Beckmann, Sila-Ibuprofen*, J. Med. Chem.*, **2020**, *63*, 21, 12614-12622.
9) Marian Olaru, Elena Rychagova, Sergey Ketkov, Yevhen Shynkarenko, Sergii Yakunin, Maksym V. Kovalenko, Artem Yablonskiy, Boris Andreev, Florian Kleemiss, Jens Beckmann, Matthias Vogt, A Small Cationic Organo-Copper Cluster as Thermally Robust Highly Photo- and Electro Luminescent Material, *J. Am. Chem. Soc.,* **2020**, *142*, 1, 373 – 381.
8) Dirk Schlüter, Florian Kleemiss, Malte Fugel, Enno Lork, Kunihisa Sugimoto, Simon Grabowsky, Jeffrey R. Harmer, Matthias Vogt, Non-Oxido-Vanadium(IV) Metalloradical Complexes with Bidentate 1,2 - Dithienylethene Ligands: Observation of Reversible Cyclization of the Ligand Scaffold in Solution, *Chem. Eur. J.,* **2020**, *26*, 6, 1335-1343.
7) Hikaru Yanai, Takumi Suzuki, Florian Kleemiss, Haruhiko Fukaya, Yasuo Dobashi, Lorraine A. Malaspina, Simon Grabowsky, Takashi Matsumoto, Chemical Bonding in Polarised Push-Pull Ethylenes, *Angew. Chem. Int. Ed.,* **2019**, *58*, 8839-8844.
6) Emanuel Hupf, Lorraine A. Malaspina, Sebastian Holsten, Florian Kleemiss, Alison J. Edwards, Jason R. Price, Valeri Kozich, Karsten Heyne, Stefan Mebs, Simon Grabowsky,

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Jens Beckmann, Proximity Enforced Agostic Interactions Involving Closed-Shell Coinage Metal Ions, *Inorg. Chem.,* **2019**, *58,* 16372 – 16378.

5) Lorraine A. Malaspina, Erna K. Wieduwilt, Justin Bergmann, Florian Kleemiss, Benjamin Meyer, Manuel F. Ruiz-López, Rumpa Pal, Emanuel Hupf, Jens Beckmann, Ross O. Piltz, Alison J. Edwards, Simon Grabowsky, Alessandro Genoni, Fast and Accurate Quantum Crystallography: From Small to Large, from Light to Heavy, *J. Phys. Chem. Lett.,* **2019**, *20*, 10, 6973-6982.

4) Malte Fugel, Maksym V. Ponomarenko, Maxie F. Hesse, Lorraine A. Malaspina, Florian Kleemiss, Kunihisa Sugimoto, Alessandro Genoni, Gerd-Volker Röschenthaler, Simon Grabowsky, Complementary bonding analysis of the N-Si interaction in pentacoordinated silicon compounds using quantum crystallography, *Dalton. Trans.,* **2019**, *48*, 16330-16339.
3) Malte Fugel, Florian Kleemiss, Lorraine A. Malaspina, Rumpa Pal, Peter R. Spackman, Dylan Jayatilaka, Simon Grabowsky, Investigating the Resonance in Nitric Acid and the Nitrate Anion Based on a Modern Bonding Analysis, *Aust. J. Chem.,* **2018**, *71*, 4, 227-237.
2) Markus Rohdenburg, Martin Mayer, Max Grellmann, Carsten Jenne, Tobias Borrmann, Florian Kleemiss, Vladimir A. Azov, Knut R. Asmis, Simon Grabowsky, Jonas Warneke, Superelectrophilic Behavior of an Anion Demonstrated by the Spontaneous Binding of Noble Gases to $[B_{12}Cl_{11}]^-$, *Angew. Chem. Int. Ed.,* **2017**, *56*, 7980-7985.
1) Nikolay A. Pushkarevsky, Pavel A. Petrov, Denis S. Grigoriev, Anton I. Smolentsev, Lucia M. Lee, Florian Kleemiss, Georgy E. Salnikov, Sergey N. Konchenko, Ignacio Vargas-Baca, Simon Grabowsky, Jens Beckmann, Andrey V. Zibarev, The Nature of Bonding in Donor-Acceptor Interactions Exemplified by Complexes of N-Heterocyclic Carbenes with 1,2,5-Telluradiazoles, *Chem. Eur. J.,* **2017**, *23*, 46, 10987-10991.

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