

## Curriculum Vitae

### Personal Information

Name **Dr. Maren Podewitz**  
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and Theoretical Chemistry,  
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### Research Interests

*Multiscale Modelling in Computational Catalysis and Material Science for Predictive Chemistry:* understanding reactivity and structure formation in catalysis and in complex (biomolecular) systems by using a broad range of methodologies from molecular dynamics to (*ab initio*) quantum chemistry.

### Education

01.2008 – 12.2010 PhD in Theoretical Chemistry, Advisor: Prof. Dr. M. Reiher, Laboratory of Physical Chemistry, ETH Zürich, Switzerland  
10.2002 – 10.2007 Bachelor and Master of Science in Chemistry (Diplomchemikerin) (grade: excellent), Friedrich-Schiller-University, Jena, Germany  
08.2005 – 07.2006 Studies of Theoretical and Physical Chemistry, Gothenburg University, Gothenburg, Sweden  
08.1995 – 06.2002 Abitur (A-levels) Albert-Einstein-Gymnasium (grade: excellent), Buchholz in der Nordheide, Germany

### Professional Experience

Since 01.2021 *Junior Group Leader*, University of Innsbruck, Austria; supervisor of independent research projects in computational chemistry, national and international collaboration with experimental chemists, supervision of master's and PhD theses  
Since 03.2020 *External Lecturer*, Management Center Innsbruck (University of Applied Sciences), Innsbruck, Austria  
05.2017 – 04.2021 *Lise Meitner Fellow*, University of Innsbruck, Austria  
08.2020 – 09.2020 *Research Stay* in the group of Prof. Dr. L. González, University of Vienna, Austria; joint project in theoretical chemistry  
08.2014 – 11.2019 *University Assistant (PostDoc)* in the group of Prof. Dr. K. R. Liedl, University of Innsbruck, Austria; supervisor of research projects in computational chemistry, supervision of bachelor's and master's theses, co-advisor of PhD theses  
08.2012 – 07.2014 *Quantitative Risk Analyst (non-academic position, career break)*, life insurance, PAX Lebensversicherungs-Gesellschaft AG, Basel, Switzerland; quantitative risk management, modelling of market risks in MATLAB, development and implementation of quantitative measures based on statistical analysis and machine learning to estimate the financial risk of assets  
08.2011 – 07.2012 *Postdoctoral Scholar* in the group of Prof. Dr. K. N. Houk, University of California Los Angeles, USA; research projects in enzyme design and physical-organic chemistry

- 01.2008 – 07.2011 *Research Assistant* in the group of Prof. Dr. M. Reiher, ETH Zürich, Switzerland; research projects in bioinorganic and theoretical chemistry, supervision of student research projects, teaching assistance
- 01.2007 – 04.2007 *Tutor* at the Friedrich-Schiller-University, Jena, Germany; supervision of laboratory work in physical and analytical chemistry, evaluation of lab reports; teaching assistant for biology students

### Grant and Scholarship Acquisition

- 2021 – 2023 Austrian Science Fund (FWF) Stand Alone Project, EUR 242.204, PI
- 2017 – 2021 Lise Meitner Fellowship of the Austrian Science Fund (FWF) for postdoctoral research, EUR 161.220, PI
- 2016 – 2018 Tyrolean Science Fund TWF, EUR 12.000, PI
- 2012 GAIN travel grant, EUR 1.000
- 2011 – 2012 Fellowship of the German Academic Exchange Service (DAAD) for postdoctoral research, EUR 40.000
- 2011 Scholarship of the Swiss National Science Foundation (SNF) for prospective researchers (declined, incompatible with DAAD fellowship) CHF 50.000
- 2009 ETH Zürich travel grant, CHF 2.000
- 2004 – 2007 Scholarship of the German Academic Scholarship Foundation (Studienstiftung des deutschen Volkes), EUR 10.000
- 2002 – 2004 Scholarship for bachelor studies of the “Fond der Chemischen Industrie”, EUR 9.900

### Prizes and Awards

- 2019 Best oral presentation award, International Symposium on Olefin Metathesis and Related Chemistry (ISOM 23), Barcelona Spain.
- 2005 Award for outstanding performance, BSc. Chemistry, German Chemical Society, Division Jena, Germany
- 2002 1<sup>st</sup> prize Youth Research Competition (Jugend Forscht), national level  
Special Award Youth Research Competition (Jugend Forscht), federal level

### Languages

German	native
English	fluent
Swedish	good
French	basic
Spanish	basic

### Teaching Experience

- Since 2020 *Lecturer:* Advanced Catalysis, MSc. Environmental, Process & Energy Engineering, Management Center Innsbruck (University of Applied Sciences), Innsbruck, Austria
- Since 2016 *Lecturer:* Methods in Theoretical Chemistry, BSc Chemistry, University of Innsbruck, Austria
- Since 2016 *Substitute Lecturer:* Theoretical Chemistry II (Quantum Chemistry), BSc. Chemistry (sporadic engagement), University of Innsbruck, Austria
- Since 2015 *Head:* Course in Theoretical Chemistry, BSc. Chemistry, University of Innsbruck, Austria
- 2015 – 2017 *Course Leader:* Advanced Laboratory Course in Theoretical Chemistry, MSc. Chemistry, University of Innsbruck, Austria

Since 2015	<i>Course Leader:</i> Visualization in Theoretical Chemistry, MSc Chemistry for High School Teachers (sporadic engagement), University of Innsbruck, Austria
2008 – 2011	<i>Teaching Assistant:</i> quantum chemistry, quantum mechanics, general and physical chemistry, ETH Zürich, Switzerland
2007	<i>Tutor:</i> Supervision of laboratory work in physical and analytical chemistry, teaching exercise classes for biology students, Friedrich-Schiller-University, Jena, Germany

### Supervision of Students

Advisor of 6 bachelor's theses (fully responsible for content), advisor of 5 master's theses (fully responsible for content), co-advisor of 3 PhD theses (one fully responsible for content), University of Innsbruck, Austria; Advisor of 5 student research projects, ETH Zürich, Switzerland

### Scientific Contributions

<b>Paper</b>	44 contributions: 42 peer reviewed articles, 1 book chapter, 1 conference proceeding
<b>Talks</b>	23 talks (plus 1 upcoming): 15 invited talks and 8 contributed talks at international conferences and seminars
<b>Posters</b>	21 poster presentations at international conferences and workshops

### Professional Service

Representative	Search Committee "Professor for Organometallic Chemistry", University of Innsbruck; Hiring and Appeal Committee "MSCA COFUND Doctoral Programme: Dynamics of Complex Continua", University of Innsbruck
Reviewer	Angew. Chem. Int. Ed., Catal. Sci. Technol., ChemCatChem, Dalton Trans., Inorg. Chim. Acta, Organometallics, Org. Biomol. Chem, J. Phys. Chem A
Co-Organizer	56 <sup>th</sup> Symposium for Theoretical Chemistry 2020, Innsbruck (cancelled due to COVID-19)
Member	GÖCH, GDCh, AGTC

### Main Collaboration Partners

Since 2018	Prof. Dr. Ivan Castillo, Universidad Nacional Autónoma de México, Mexico
Since 2017	Prof. Dr. Michael R. Buchmeiser, University of Stuttgart, Germany
Since 2017	Prof. Dr. Benno Bildstein, University of Innsbruck, Austria
Since 2016	Dr. Jörn Bruns, University of Cologne, Germany
Since 2015	Prof. Dr. Bernhard Kräutler, University of Innsbruck, Austria

### Extracurricular and Outreach Activities

Since 2016	"Lange Nacht der Forschung", University of Innsbruck
Since 2015	"Junge Uni", University of Innsbruck
2006 – 2007	Mentor for exchange students, Friedrich-Schiller-University, Jena, Germany
2005 – 2006	"Peer helper" training, Gothenburg University, Gothenburg, Sweden
2004 – 2005	Elected member of the chemistry student representatives Friedrich-Schiller-University, Jena, Germany
1996–2002	Trainer for Judo, VfL Jesteburg, Germany

**List of Acquired Third-Party Funds**

2021 – 2023	Stand Alone FWF Project: “Reactivity and Selectivity in Olefin Metathesis – Predicting Catalysis by Quantum Chemistry” (PI)	EUR 242.204
2017 – 2021	Lise Meitner Program of the FWF: “Vitamin B <sub>12</sub> derivatives as potential antivitamin: understanding their function as antimetabolites” (personal grant)	EUR 161.220
2016 – 2018	Tyrolean Science Fund (TWF): “Vitamin B <sub>12</sub> derivatives as potential antivitamin: understanding their function as antimetabolites” (PI)	EUR 12.000
2012	GAIN Travel Grant	EUR 1.000
2011 – 2012	Fellowship of the German Academic Exchange Service (DAAD) for postdoctoral research (personal grant)	EUR 40.000
2011	Scholarship of the Swiss National Science Foundation (SNF) for prospective researchers (declined, incompatible with DAAD fellowship) (personal grant)	EUR 40.000 (CHF 50.000)
2009	ETH Zürich Travel Grant	EUR 1.750 (CHF 2.000)
2004 – 2007	Scholarship of the German Academic Scholarship Foundation (Studienstiftung des deutschen Volkes)	EUR 10.000
2002 – 2004	Scholarship for Bachelor Studies of the “Fond der Chemischen Industrie”	EUR 9.900

**Total: ca. 520.000 €**

## Peer-Reviewed Publications

\* Corresponding author

[OA]: Open Access

## Accepted

1. Patrick K. Quoika, Monica L. Fernández-Quintero, Maren Podewitz, Florian Hofer, Klaus R. Liedl. "Implementation of the Freely Jointed Chain Model to Assess Kinetics and Thermodynamics of Thermosensitive Coil-Globule Transition by Markov States", *Journal of Physical Chemistry B* (2021), *accepted*.
2. Chengjie Li, Maren Podewitz\*, Bernhard Kräutler. "A Blue Zinc-Complex of a Dioxobilin-Type Pink Chlorophyll Catabolite Exhibiting Bright Chelation-Enhanced Red Fluorescence", *European Journal of Inorganic Chemistry* (2021), *accepted*. DOI: 10.1002/ejic.202100206.

## Published

3. [OA] Miguel Steiner, Tanja Holzknacht, Michael Schauerl, Maren Podewitz\*. "Quantum Chemical Microsolvation by Automated Solvent Placement", *Molecules*, **26** (2021), 1793. DOI: 10.3390/molecules26061793 Part of the Special Issue: Describing Bulk Phase Effects with Ab Initio Methods.
4. [OA] Franz-Lucas Haut, Christoph Habiger, Lukas Anton Wein, Klaus Wurst, Maren Podewitz\*, Thomas Magauer\*. "Rapid Assembly of Tetrasubstituted Furans via Pummerer-type Rearrangement", *Journal of the American Chemical Society*, **143** (2021), 1216–1223. DOI: 10.1021/jacs.0c12194. IF: 14.6.
5. [OA] Leonard C. Pasqualini, Oliver Janka, Selina Olthof, Hubert Huppertz, Klaus R. Liedl, Rainer Pöttgen, Maren Podewitz\*, Jörn Bruns\*. "Ni[B<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>] and Co[B<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>]: Unveiling systematic trends in phyllosilicate borosulfates", *Chemistry – A European Journal*, **26** (2020), 17405-17415. DOI: 10.1002/chem.202002221. IF: 4.9.
6. [OA] Dennis F. Dinu, Maren Podewitz, Hinrich Grothe, Thomas Loerting, Klaus R. Liedl. "On the Synergy of Matrix-Isolation Infrared Spectroscopy and Vibrational Configuration Interaction Computations", *Theoretical Chemistry Accounts*, **139** (2020), 174. DOI: 10.1007/s00214-020-02682-0. IF: 1.5.
7. [OA] Christoph Kieninger, Klaus Wurst, Maren Podewitz, Evelyne Deery, Andrew D Lawrence, Klaus R Liedl, Martin J Warren, Bernhard Kräutler. "Replacement of the Cobalt-Center of Vitamin B<sub>12</sub> by Nickel – Nibalamin and Related Ni(II)-Corrins Prepared from Hydrogenobalamin and Other Metal-Free B<sub>12</sub>-Ligands", *Angewandte Chemie International Edition*, **132** (2020), 20304-203011. DOI: 10.1002/anie.202008407. IF: 13.0.
8. [OA] Patrick K. Quoika, Maren Podewitz, Yin Wang, Anna S. Kamenik, Johannes R. Loeffler, Klaus R. Liedl. "Thermosensitive Hydration of Four Acrylamide-Based Polymers in Coil and Globule Conformations", *Journal of Physical Chemistry B*, **124** (2020), 9745-9756. DOI: 10.1021/acs.jpcc.0c07232. IF: 2.9.
9. [OA] Sina K. Goetzfried, Caroline Gallati, Monika Cziferszky, Radu A. Talmazan, Klaus Wurst, Klaus R. Liedl, Maren Podewitz\*, Ronald Gust\*. "N-Heterocyclic Carbene Gold(I) Complexes: Mechanism of the Ligand Scrambling Reaction and their Oxidation to Gold(III) in Aqueous Solutions", *Inorganic Chemistry*, **59** (2020), 15312-15232. DOI: 10.1021/acs.inorgchem.0c02298. IF: 4.8.
10. [OA] Matthias Schmid, Kevin Rafael Sokol, Lukas Anton Wein, Sofia Torres Venegas, Christina Meisenbichler, Klaus Wurst, Maren Podewitz, Thomas Magauer. "Synthesis of Vicinal Quaternary

- All-Carbon Centers via Acid-catalyzed Cycloisomerization of Neopentyl Epoxides”, *Organic Letters*, **22** (2020), 6526-6531. DOI: 10.1021/acs.orglett.0c02296. IF: 6.1.
11. [OA] Dennis F. Dinu, Maren Podewitz, Hinrich Grothe, Thomas Loerting, Klaus R. Liedl. “Decomposing anharmonicity and mode-coupling from matrix effects in the IR spectra of matrix-isolated carbon dioxide and methane”, *Physical Chemistry Chemical Physics*, **22** (2020), 17932-17947. DOI: 10.1039/d0cp02121k. IF: 3.4.
  12. [OA] Radu A. Talmazan, Klaus R. Liedl, Bernhard Kräutler, Maren Podewitz\*. “The intermolecular anthracene-transfer in a regiospecific antipodal C<sub>60</sub> difunctionalization”, *Organic & Biomolecular Chemistry*, **18** (2020), 4090-4103. DOI: 10.1039/d0ob00520g. IF: 3.4.
  13. [OA] Eva-Maria Köck, Jürgen Bernard, Maren Podewitz, Dennis F. Dinu, Roland G. Huber, Klaus R. Liedl, Hinrich Grothe, Erminald Bertel, Robert Schlögl, Thomas Loerting. “Alpha carbonic acid revisited Carbonic acid monomethyl ester as a solid and its conformational isomerism in the gas phase”, *Chemistry – A European Journal*, **26** (2020), 285-305. DOI: 10.1002/chem.201904142. IF: 4.9.
  14. [OA] Dennis F. Dinu, Benjamin Ziegler, Maren Podewitz, Klaus R. Liedl, Thomas Loerting, Hinrich Grothe, Guntram Rauhut. “The Interplay of VSCF/VCI calculations and Matrix-Isolation IR Spectroscopy - Mid Infrared Spectrum of CH<sub>3</sub>CH<sub>2</sub>F and CD<sub>3</sub>CD<sub>2</sub>F”, *Journal of Molecular Spectroscopy*, **367** (2020), 111224. DOI: 10.1016/j.jms.2019.111224. IF: 1.2.
  15. [OA] Elisabeth Selb, Lisa Declara, Lkhamsuren Bayarjargal, Maren Podewitz, Martina Tribus, Gunther Heymann. “Crystal Structure and Properties of a UV-transparent High-Pressure Polymorph of Mg<sub>3</sub>TeO<sub>6</sub> with Second Harmonic Generation Response”, *European Journal of Inorganic Chemistry*, **43** (2019), 4668-4676. DOI: 10.1002/ejic.201900998. IF: 2.5.
  16. Maren Podewitz,<sup>+</sup> Yin Wang,<sup>+</sup> Patrick K. Quoika, Johannes R. Loeffler, Michael Schauerl, Klaus R. Liedl. “Coil-Globule Transition Thermodynamics of Poly(N-isopropylacrylamide)”, *Journal of Physical Chemistry B*, **123** (2019), 8838-8847. DOI: 10.1021/acs.jpcc.9b06125. <sup>+</sup>equally contributed. IF: 2.9.
  17. [OA] Dennis F. Dinu, Maren Podewitz, Hinrich Grothe, Klaus R. Liedl, Thomas Loerting. “Toward Elimination of Discrepancies Between Theory and Experiment: Anharmonic Rotational-Vibrational Spectrum of Water in Solid Noble Gas Matrices”, *Journal of Physical Chemistry A*, **123** (2019), 8234-8242. DOI: 10.1021/acs.jpca.9b07221. IF: 2.6.
  18. [OA] Christoph Kieninger,<sup>+</sup> Joseph A. Baker,<sup>+</sup> Maren Podewitz,<sup>+</sup> Klaus Wurst, Stefan Jokusch, Andrew D. Lawrence, Evelyne Deery, Karl Gruber, Klaus R. Liedl, Martin J. Warren, Bernhard Kräutler. “Zinc Substitution of Cobalt in Vitamin B<sub>12</sub> - Zincobyrinic acid and Zincobalamin as Luminescent Structural B<sub>12</sub>-Mimics”, *Angewandte Chemie International Edition*, **58** (2019), 14568–14572. DOI:10.1002/anie.201908428. <sup>+</sup>equally contributed. IF: 13.0.
  19. [OA] Christoph Kieninger,<sup>+</sup> Evelyne Deery,<sup>+</sup> Andrew D. Lawrence,<sup>+</sup> Maren Podewitz,<sup>+</sup> Klaus Wurst, Emi Nemoto-Smith, Florian J. Widner, Joseph A. Baker, Steffen Jockusch, Christoph R. Kreutz, Klaus R. Liedl, Karl Gruber, Martin J. Warren, Bernhard Kräutler. “The Corrin Ligand is a Molecular Entatic State Module Evolved to Enhance Catalysis by B<sub>12</sub>-Cofactors”, *Angewandte Chemie International Edition*, **58** (2019), 10756–10760. DOI: 10.1002/anie.201904713. <sup>+</sup>equally contributed. IF: 13.0.
  20. [OA] Katharina Herz, Maren Podewitz\*, Laura Stöhr, Dongren Wang, Wolfgang Frey, Klaus R. Liedl, Suman Sen, Michael R. Buchmeiser\*. “Mechanism of Olefin Metathesis with Neutral and Cationic Molybdenum Imido Alkylidene N Heterocyclic Carbene”, *Journal of the American Chemical Society*, **141** (2019), 8264–8276. DOI: 10.1021/jacs.9b02092. First Corresponding Authorship on a JACS Paper of the Institute of Theoretical Chemistry since 2010. IF: 14.6.
  21. [OA] Theresia Erhart, Cecilia Mittelberger, Xiujun Liu, Maren Podewitz, Chengjie Li, Gerhard Scherzer, Gertrud Stoll, Josep Valls, Peter Robatscher, Klaus R. Liedl, Michael Oberhuber, Bernhard

- Kräutler. “Novel Types of Hypermodified Fluorescent Phyllobilins from Breakdown of Chlorophyll in Senescent Leaves of Grapevine (*Vitis vinifera*)”, *Chemistry – A European Journal*, **24** (2018), 17268-17279. DOI: 10.1002/chem.201803128. IF: 4.9.
22. [OA] Steffen Spieler, Dennis F. Dinu, Pavol Jusko, Björn Bastian, Malcolm Simpson, Maren Podewitz, Klaus R. Liedl, Stephan Schlemmer, Sandra Brünken, Roland Wester. “Low Frequency Vibrational Anharmonicity and Nuclear Spin Effects of Cl(H<sub>2</sub>) and Cl(D<sub>2</sub>)”, *Journal of Chemical Physics*, **149** (2018), 17310. DOI: 10.1063/1.5049680. IF: 3.0.
23. Maren Podewitz,<sup>+</sup> Yin Wang,<sup>+</sup> Paraskevi Gkeka, Susanne von Grafenstein, Klaus R. Liedl, Zoe Cournia. “Phase Diagram of a Stratum Corneum Lipid Mixture”, *Journal of Physical Chemistry B*, **122** (2018), 10505-10521. DOI: 10.1021/acs.jpcc.8b07200. <sup>+</sup>equally contributed. IF: 2.9.
24. [OA] Birgit J. Waldner, Johannes Kraml, Ursula Kahler, Alexander Spinn, Michael Schauerl, Maren Podewitz, Julian E. Fuchs, Gabriele Cruciani, Klaus R. Liedl. “Electrostatic Recognition in Substrate Binding to Serine Proteases”, *Journal of Molecular Recognition*, **31** (2018), e2727. DOI: 10.1002/jmr2727. IF: 1.9.
25. [OA] Jörn Bruns, Maren Podewitz, Klaus R. Liedl, Oliver Janka, Rainer Pöttgen, Hubert Huppertz. “Cu[B<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>] and Cu[B(SO<sub>4</sub>)<sub>2</sub>(HSO<sub>4</sub>)]—Two Silicate Analogue Borosulfates Differing in their Dimensionality: A Comparative Study of Stability and Acidity”, *Angewandte Chemie International Edition*, **57** (2018), 9548-9552. DOI:10.1002/anie.201803395 and DOI:10.1002/ange.201803395. IF: 13.0.
26. [OA] Stefan Vanicek, Maren Podewitz, Jessica Stubbe, Dennis Schulze, Holger Kopacka, Klaus Wurst, Thomas Müller, Petra Lippmann, Simone Haslinger, Herwig Schottenberger, Klaus R. Liedl, Ingo Ott, Biprajit Sarkar, Benno Bildstein. “Highly Electrophilic, Catalytically Active and Redox-Responsive Cobaltoceniumyl and Ferrocenyl Triazolylidene Coinage Metal Complexes”, *Chemistry – A European Journal*, **24** (2018), 3742-3753. DOI: 10.1002/chem.201705051. IF: 4.9.
27. [OA] Stefan Vanicek, Maren Podewitz, Christopher Hassenrück, Michael Pittracher, Holger Kopacka, Klaus Wurst, Thomas Müller, Klaus R. Liedl, Rainer F. Winter, Benno Bildstein. “Cobaltocenyliene: A Mesoionic Metallocene Carbene, Stabilized in a Gold (III) Complex”, *Chemistry – A European Journal*, **24** (2018), 3165-3169. DOI: 10.1002/chem.201800147. IF: 4.9.
28. [OA] Chengjie Li, Klaus Wurst, Joachim Berghold, Maren Podewitz, Klaus R. Liedl, Bernhard Kräutler. “Pyro-Phyllobilins: Elusive Chlorophyll Catabolites Lacking a Critical Carboxylate Function of the Natural Chlorophylls”, *Chemistry – A European Journal*, **24** (2018), 2987-2998. DOI: 10.1002/chem.201705331. IF: 4.9.
29. Jörn Bruns, Maren Podewitz, Michael Schauerl, Bastian Joachim, Klaus R. Liedl, Hubert Huppertz. “CaB<sub>2</sub>S<sub>4</sub>O<sub>16</sub>: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology”, *Chemistry – A European Journal*, **23** (2018), 16773-16781. DOI: 10.1002/chem.201704228. IF: 4.9.
30. Martin K. Schmitt, Maren Podewitz, Klaus R. Liedl, Hubert Huppertz. “High-Pressure Synthesis and Characterization of the Ammonium Yttrium Borate (NH<sub>4</sub>)YB<sub>8</sub>O<sub>14</sub>”, *Inorganic Chemistry*, **56** (2018), 14291-14299. DOI: 10.1021/acs.inorgchem.7b02402. IF: 4.8.
31. [OA] Michael Schauerl, Maren Podewitz, Teresa S. Ortner, Franz Waibl, Alexander Thoeny, Thomas Loerting, Klaus R. Liedl. “Balance Between Hydration Enthalpy and Entropy is Important for Ice Binding Surfaces in Antifreeze Proteins”, *Scientific Reports*, **7** (2017), 11901. DOI:10.1038/s41598-017-11982-8. IF: 4.0.
32. Jörn Bruns, Maren Podewitz, Michael Schauerl, Klaus R. Liedl, Oliver Janka, Rainer Pöttgen, Hubert Huppertz. “Ag[B(SO<sub>4</sub>)<sub>2</sub>] – Synthesis, crystal structure, and characterization of the first precious metal borosulfate”, *European Journal of Inorganic Chemistry*, **23** (2017), 16773-16781. DOI: 10.1002/ejic.20170036. IF: 2.5.

33. [OA] Michael Schauerl, Paul Czodrowski, Julian E. Fuchs, Roland G. Huber, Birgit J. Waldner, Maren Podewitz, Christian Kramer, Klaus R. Liedl. "A Binding Pose Flip Explained via Enthalpic and Entropic Contributions", *Journal of Chemical Information and Modeling*, **57** (2017), 345-354, DOI: 10.1021/acs.jcim.6b00483. IF: 4.5.
34. [OA] Chengjie Li, Klaus Wurst, Steffen Jokusch, Karl Gruber, Maren Podewitz, Klaus R. Liedl, Bernhard Kräutler. "Chlorophyll-Derived Yellow Phyllobilins of Higher Plants as Medium-Responsive Chiral Photoswitches", *Angewandte Chemie International Edition*, **55** (2016), 15760-15765. DOI: 10.1002/anie.201609481. IF: 13.0.
35. [OA] Michael Schauerl, Maren Podewitz, Birgit J. Waldner, Klaus R. Liedl. "Enthalpic and Entropic Contributions to Hydrophobicity", *Journal of Chemical Theory and Computation*, **12** (2016), 4600–4610, DOI: 10.1021/acs.jctc.6b00422. IF: 5.0.
36. Christian Kramer, Maren Podewitz, Peter Ertl, Klaus R. Liedl. "Unique Macrocycles in the Taiwan Traditional Chinese Medicine Database", *Planta Medica*, **81** (2015), 459-466. DOI:10.1055/s-0035-1545881. IF: 2.7.
37. Maren Podewitz, Martin T. Stiebritz, Markus Reiher. "An Enquiry into Theoretical Bioinorganic Chemistry: How Heuristic is the Character of Present-Day Quantum Chemical Methods?", *Faraday Discussions*, **148** (2011), 119–135. DOI: 10.1039/C004195E. IF 3.8.
38. Maren Podewitz, Markus Reiher. "Spin Interactions in Cluster Chemistry", *Advances in Inorganic Chemistry*, **62** (2010), 177–230. DOI:10.1016/S0898-8838(10)62005-3. IF: 2.5.
39. Maren Podewitz, Jacco D. van Beek, Michael Wörle, Tobias Ott, Daniel Stein, Heinz Rügger, Beat H. Meier, Markus Reiher, Hansjörg Grützmacher. "Ion Dynamics in Confined Spaces: Sodium Ion Mobility in Icosahedral Container Molecules", *Angewandte Chemie International Edition*, **49** (2010), 7465–7469. DOI: 10.1002/ange.201003441. IF: 13.0.
40. Astrid Malassa, Christina Agthe, Helmar Görls, Maren Podewitz, Lian Yu, Carmen Herrmann, Markus Reiher, Matthias Westerhausen. "Synthesis, Structures and Magnetic Properties of N-Trialkylsilyl-8-amidoquinoline Complexes of Chromium, Manganese, Iron, and Cobalt as well as of Wheel-like Hexa-nuclear Iron(II) and Manganese(II) Bis(8-Amidoquinoline)", *European Journal of Inorganic Chemistry*, **12** (2010), 1777–1790. IF: 2.5.
41. Carmen Herrmann, Maren Podewitz, Markus Reiher. "Restrained Optimization of Broken-Symmetry Determinants", *International Journal of Quantum Chemistry*, **109** (2009), 2430–2446. IF: 1.7.
42. Maren Podewitz, Carmen Herrmann, Astrid Malassa, Matthias Westerhausen, Markus Reiher. "Spin-Spin Interactions in Polynuclear Transition-Metal Complexes", *Chemical Physics Letters*, **451** (2008), 301–308. DOI:10.1016/j.cplett.2007.12.011. IF: 2.0.



### Book Chapters

1. Maren Podewitz, Thomas Weymuth, Markus Reiher. “Density Functional Theory for Transition Metal Chemistry: The Case of a Water Splitting Ruthenium Cluster”, Modeling Molecular Properties, Ed. P. Comba (2011), 139–163.

### Conference Proceedings

1. Maren Podewitz, Bernhard Kräutler, Klaus R. Liedl. “Understanding and Improving B-12 Antivitamins By Computational Studies”, 8th International Conference on Biological Inorganic Chemistry (ICBIC) Location: Florianopolis, Brazil Date: JUL 31-AUG 04, 2017, *Journal of Biological Inorganic Chemistry*, **22**(1), S48.

### Journal Covers

1. Cover Picture: Ni[B<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>] and Co[B<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>]: Unveiling systematic trends in phyllosilicate borosulfates (Chem. Eur. J. (2020))., Leonard Pasqualini, Oliver Janka, Selina Olthof, Hubert Huppertz, Klaus R. Liedl, Rainer Pöttgen, Maren Podewitz\*, Jörn Bruns\*. DOI: 10.1002/chem.202003298.
2. Cover Feature: Toward Elimination of Discrepancies Between Theory and Experiment: Anharmonic Rotational-Vibrational Spectrum of Water in Solid Noble Gas Matrices. Dennis F. Dinu, Maren Podewitz, Hinrich Grothe, Klaus R. Liedl, Thomas Loerting. (J. Chem. Phys. A 123/2019). [https://pubs.acs.org/pb-assets/images/\\_journalCovers/jpcaf/h/jpcaf\\_h\\_v123i038-2.jpg?0.6043850775677858](https://pubs.acs.org/pb-assets/images/_journalCovers/jpcaf/h/jpcaf_h_v123i038-2.jpg?0.6043850775677858).
3. Inside Cover: Cu[B<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>] and Cu[B(SO<sub>4</sub>)<sub>2</sub>(HSO<sub>4</sub>)]—Two Silicate Analogue Borosulfates Differing in their Dimensionality: A Comparative Study of Stability and Acidity (Angew. Chem. Int. Ed. 30/2018), Jörn Bruns, Maren Podewitz, Klaus R. Liedl, Oliver Janka, Rainer Pöttgen, Hubert Huppertz. DOI: 10.1002/anie.201805347.
4. Cover Feature: Highly Electrophilic, Catalytically Active and Redox-Responsive Cobaltoceniumyl and Ferrocenyl Triazolylidene Coinage Metal Complexes (Chem. Eur. J. 15/2018). Stefan Vanicek, Maren Podewitz, Jessica Stubbe, Dennis Schulze, Holger Kopacka, Klaus Wurst, Thomas Müller, Petra Lippmann, Simone Haslinger, Herwig Schottenberger, Klaus R. Liedl, Ingo Ott, Biprajit Sarkar, Benno Bildstein. DOI: 10.1002/chem.201800112.
5. Frontispiece: CaB<sub>2</sub>S<sub>4</sub>O<sub>16</sub>: A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. (Chemistry – Eur. J. 23/2017) Jörn Bruns, Maren Podewitz, Michael Schauerl, Bastian Joachim, Klaus R. Liedl, Hubert Huppertz. DOI: 10.1002/chem.201786664.
6. Front Cover: Ag[B(SO<sub>4</sub>)<sub>2</sub>]-Synthesis, Crystal Structure, and Characterization of the First Precious-Metal Borosulfate (Eur. J. Inorg. Chem. 34/2017). Jörn Bruns, Maren Podewitz, Michael Schauerl, Klaus R. Liedl, Oliver Janka, Rainer Pöttgen, Hubert Huppertz. DOI: 10.1002/ejic.201700916.
7. Front Cover: A Binding Pose Flip Explained via Enthalpic and Entropic Contributions. (J. Chem. Inf. Model. 57(2), 2017). Michael Schauerl, Paul Czodrowski, Julian E. Fuchs, Roland G. Huber, Birgit J. Waldner, Maren Podewitz, Christian Kramer, Klaus R. Liedl. <https://pubs.acs.org/toc/jcisd8/57/2>.
8. Inside Cover: Chlorophyll-Derived Yellow Phyllobilins of Higher Plants as Medium-Responsive Chiral Photoswitches (Angew. Chem. Int. Ed. 51/2016). Chengjie Li, Klaus Wurst, Steffen Jokusch, Karl Gruber, Maren Podewitz, Klaus R. Liedl, Bernhard Kräutler. DOI: 10.1002/anie.201611033.

**Non-peer reviewed publications**

1. “Neue Bausteine für die Synthese” Newsroom University of Innsbruck, 2020, <https://www.uibk.ac.at/newsroom/neue-bausteine-fuer-die-synthese.html.de>
2. “Ein Herz au Nickel, Newsroom University of Innsbruck, 2020, <https://www.uibk.ac.at/newsroom/ein-herz-aus-nickel.html.de>
3. “Spiel mit den chemischen Elementen”, Newsroom University of Innsbruck, 2019, <https://www.uibk.ac.at/newsroom/spiel-mit-den-chemischen-elementen.html.de>.
4. “Forschungsprojekte am Vienna Scientific Cluster“, Brochure, 2018, [http://vsc.ac.at/fileadmin/user\\_upload/vsc/documents/download/VSC-brochure-2018-FP-web.pdf](http://vsc.ac.at/fileadmin/user_upload/vsc/documents/download/VSC-brochure-2018-FP-web.pdf).
5. “Neue „Enkel“ einer prähistorischen Substanz” Newsroom University of Innsbruck, 2018, <https://www.uibk.ac.at/newsroom/neue-enkel-einer-praehistorischen-substanz.html.de>

## Talks

### Upcoming

1. Title to be determined, 12<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists, July 3-8, 2022, Vancouver, Canada (**invited**).

### Past

2. "Towards predictive chemistry by multiscale modelling", Hearing for an assistant professorship position, TU Wien, March 15, 2021, Vienna, Austria, *online via Zoom* (**invited**).
3. "Modelling Chemical and Physical Properties of Complex Systems", Hearing for an assistant professorship position, TU Graz, January 15, 2021, Graz, Austria, *online via Webex* (**invited**).
4. "Reaction Mechanisms and Reactivity of Complex Systems Uncovered by Computational Chemistry", Seminar of the Physical-Chemical Society (CPG), TU Wien, January 12, 2021, Vienna, Austria, *online via Zoom* (**invited**).
5. "Unravelling Reaction Mechanisms and Reactivity of Complex Systems by Computational Chemistry", Institute seminar, Karl-Franzens University Graz, November 20, 2020, Graz, Austria, *online via Zoom* (**invited**).
6. "Unravelling Reaction Mechanisms and Reactivity of Complex Systems by Computational Chemistry", 8<sup>th</sup> Carnival Conference Session 2020, February 19, 2020, Cologne, Germany (**invited**).
7. "Understanding Complex Molecular Systems by Multiscale Modelling" Hearing for an assistant professorship position, Radboud University Nijmegen, January 7, 2020, Nijmegen, The Netherlands (**invited**).
8. "Towards Predictive Catalysis by Multiscale Modelling", Hearing for an assistant professorship position, Universiteit van Amsterdam, December 17, 2019, Amsterdam, The Netherlands (**invited**).
9. "Arzneimittelforschung mit Hilfe der Computerchemie", Hearing for an assistant professorship position, Institute of Pharmaceutical Chemistry, University of Innsbruck, November 8, 2019, Innsbruck, Austria (**invited**).
10. "Multiscale Modelling in Computational Catalysis", Hearing for an assistant professorship position, Institute of Ionphysics and Applied Physics, University of Innsbruck, September 16, 2019, Innsbruck, Austria (**invited**).
11. "The Mechanism of Olefin Metathesis with a Molybdenum Imido Alkylidene *N*-Heterocyclic Carbene Catalyst Investigated by Quantum Chemistry", 7<sup>th</sup> Latin American Symposium on Coordination and Organometallic Chemistry, August 27-30, 2019, Cartagena, Colombia (**invited**).
12. "Elucidating the Mechanism of Olefin Metathesis with a Molybdenum Imido Alkylidene *N*-Heterocyclic Carbene Catalyst by Quantum Chemistry", International Symposium on Olefin Metathesis and Related Chemistry, June 30-July 3, 2019, Barcelona Spain.
13. "Elucidating the Olefin Metathesis Mechanism of A Novel Cationic Molybdenum Catalyst by Quantum Chemistry", Federal University of Minas Gerais, March 21, 2019, Belo Horizonte, Brazil (**invited**).
14. "Associative or Dissociative? Elucidating the Mechanism of Olefin Metathesis with A Novel Cationic Molybdenum Catalyst by Quantum Chemistry", March 20, 2019, Federal University of Rio de Janeiro, Brazil (**invited**).
15. "Reaction Mechanism of Olefin Metathesis with a Novel Molybdenum Catalyst", Girona Seminar: Predictive Catalysis, Transition-Metal Reactivity by Design, April 3-6, 2018, Girona, Spain.

16. “Unravelling Reaction Mechanisms with Quantum Chemistry”, DK-CIM Winter School, March 4-7, 2018, Obergurgl, Austria (**invited**).
17. “A Novel Mo-Alkylidene Catalyst Facilitates Olefin Metathesis in the Presence of Functional Groups”, Polymat 2017, October 15-19, 2017, Huatulco, Mexico (**invited**).
18. “A Novel Mo-Alkylidene Catalyst Facilitates Olefin Metathesis in the Presence of Functional Groups”, October 13, 2017, National Autonomous University Mexico, Mexico City, Mexico (**invited**).
19. “Novel Mo-Alkylidene Catalysts Can Tolerate Functional Groups in Olefin Metathesis” Gordon Research Seminar: Computational Chemistry, July 2-3, 2016, Girona, Spain.
20. “Solvation and/or Dispersion: The Quest for Accurate Bond Dissociation Energies in B<sub>12</sub> Antivitamins”, Boeringer Ingelheim, November 30, 2015, Biberach, Germany.
21. “On or Off: How Conformations Influence Bond Dissociation Energies in B<sub>12</sub> Antivitamins”, 16<sup>th</sup> Austrian Chemistry Days, September 21-24, 2015, Innsbruck, Austria.
22. “Spin-Spin Interactions in Biologically Relevant Model Clusters” C4 Workshop IBM, January 19, 2011, Rüslikon, Switzerland.
23. “Understanding Structure and Reactivity of Transition-Metal Clusters”, Seminar in Theoretical Chemistry, February 23, 2010, Jerusalem, Israel.
24. “Local Spin and Bond Order Terms”, Seminar Special Topics in Theoretical Chemistry, January 21, 2009, Zürich, Switzerland.

## Posters

1. 55<sup>th</sup> Symposium for Theoretical Chemistry, 09.2019, Rostock, Germany.
2. 10<sup>th</sup> Triennial Congress of the International Society for Theoretical Chemical Physics, 07.2019, Tromsø, Norway
3. Gordon Research Seminar: Computational Chemistry, 07.2018, Mount Snow, VT, USA.
4. Gordon Research Conference: Computational Chemistry, 07.2018, Mount Snow, VT, USA.
5. 16<sup>th</sup> International Congress on Quantum Chemistry, 06.2018, Menton, France.
6. Computational Catalysis for Sustainable Chemistry, 06.2018, Tarragona, Spain.
7. 11<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), 09.2017, Munich, Germany.
8. 18<sup>th</sup> International Conference on Bioinorganic Chemistry, 07.2017, Florianopolis, Brazil.
9. FemEx Netherlands 2017, 06.2017, Putten, Netherlands.
10. Theory and Applications of Computational Chemistry, 09.2016, Seattle, USA.
11. Gordon Research Conference: Computational Chemistry, 07.2016, Girona, Spain.
12. Girona Seminar: Predictive Catalysis, 04.2016, Girona, Spain.
13. 6<sup>th</sup> Annual CMBI Meeting, 03.2016, Gnadenwald, Austria.
14. 7<sup>th</sup> Life Science Meeting, 02.2015, Innsbruck, Austria.
15. 14<sup>th</sup> International Congress on Quantum Chemistry, Satellite Meeting, 06.2012, Los Angeles, USA.

16. Faraday Discussion 148, 07.2010, Nottingham, England.
17. 14<sup>th</sup> International Conference on Bioinorganic Chemistry, 07.2009, Nagoya, Japan.
18. C4 Workshop Novartis Institutes for Biomedical Research, 01.2009, Basel, Switzerland.
19. 44<sup>th</sup> Symposium for Theoretical Chemistry STC 2008, 09.2008, Ramsau, Austria.
20. 10<sup>th</sup> Sostrup Summer School of Quantum Chemistry and Molecular Properties, 07.2008, Sostrup, Denmark.
21. Association of Young Chemists (JungChemikerForum) Frühjahrssymposium 2008, 03.2008, Rostock, Germany.