

## Curriculum Vitae

### Personal Information

Name **Dr. Maren Podewitz**  
Address Institute of General, Inorganic  
and Theoretical Chemistry,  
Innrain 80/82, 6020 Innsbruck, Austria  
Phone +43 512 507 57104  
E-Mail [maren.podewitz@uibk.ac.at](mailto:maren.podewitz@uibk.ac.at)  
Homepage <http://homepage.uibk.ac.at/~c72448/podewitz.html>

### Research Interests

*Multiscale Modelling in (Bio-)Catalysis and Biomolecular Systems*: understanding functionality and selectivity of (bio-)chemical reactions and biomolecular interfaces by means of computational chemistry using a broad range of methodologies from molecular modelling to *ab-initio* quantum chemistry. A focus is on assessing reaction mechanisms of transition-metal catalysts and elucidating structure and dynamics of biomolecules and membranes.

### Education

01.2008 – 12.2010 PhD in Theoretical Chemistry, Advisor: Prof. Dr. M. Reiher, Laboratory of Physical Chemistry, ETH Zürich, Switzerland  
Title: *Structure Determining Interactions in Polynuclear Metal Clusters*  
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 05.2017 *Lise Meitner Fellow*, University of Innsbruck, Austria; supervisor of independent research projects in computational chemistry, national and international collaboration with experimental chemists in the fields of inorganic chemistry  
since 08.2014 *University Assistant* 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, teaching  
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 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; led 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: co-led research projects in bioinorganic and theoretical chemistry, supervision of student research projects, teaching assistance

01.2007 – 04.2007 *Tutor* 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

2017–2021 Lise Meitner Fellowship of the Austrian Science Fund (FWF) for postdoctoral research, EUR 161.220

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, 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 2016 *Lecturer:* Methods in Theoretical Chemistry, BSc Chemistry curriculum, University of Innsbruck, Austria

since 2016 *Substitute Lecturer:* Theoretical Chemistry II (Quantum Chemistry), BSc Chemistry curriculum, University of Innsbruck, Austria

since 2015 *Head:* Course in Theoretical Chemistry, BSc Chemistry curriculum, University of Innsbruck, Austria

since 2015 *Course Leader:* Advanced Laboratory Course in Theoretical Chemistry, MSc Chemistry curriculum, University of Innsbruck, Austria

2015 *Course Leader:* Visualization in Theoretical Chemistry, MSc Chemistry for High School Teachers curriculum, University of Innsbruck, Austria

2008–2011 *Teaching Assistant,* ETH Zürich, Switzerland; teaching classes in quantum chemistry, quantum mechanics, general and physical chemistry

2007 *Tutor* for biology students, Friedrich-Schiller University, Jena, Germany; supervision of laboratory work in physical and analytical chemistry, teaching exercise classes

### **Supervision of Students**

Advisor of 6 bachelor's theses (1 ongoing) (fully responsible for content), advisor of 4 master's theses (2 ongoing) (fully responsible for content), co-advisor of 2 PhD theses, University of Innsbruck, Austria  
Advisor of 5 student research projects, ETH Zürich, Switzerland

### **Scientific Contributions**

**Paper** 30 contributions: 26 published peer reviewed articles (2 articles submitted), 1 book chapter, 1 conference proceeding; h-index: 8, total number of citations: 202; Google Scholar August 2019  
JACS (1), Angewandte Chemie (5), Chemistry (5)

**Talks** 15 talks: 7 invited talks and 8 contributed talks at international conferences and seminars

**Posters** 21 poster presentations at international conferences and workshops

### **Professional Service**

**Representative** Search Committee "Professor for Organometallic Chemistry", Innsbruck, Austria, 2019

**Reviewer** Inorganica Chimia Acta

**Co-Organizer** Symposium for Theoretical Chemistry 2020, Innsbruck, Austria

**Other** Member of Poster Award Jury ISOM23, Session Chair ISTCP-X

### **Main Collaboration Partners**

Since 2018 Prof. Dr. Ivan Castillo, Universidad Nacional Autónoma de México, Mexico

Since 2018 Prof. Dr. Ronaldo Nagem, Universidad de Minas Gerais, Belo Horizonte, Brazil

Since 2017 Prof. Dr. Michael R. Buchmeiser, University of Stuttgart, Germany

Since 2016 Prof. Dr. Hubert Huppertz, University of Innsbruck, Austria

Since 2015 Prof. Dr. Bernhard Kräutler, University of Innsbruck, Austria

### **Extracurricular and Outreach Activities**

Since 2016 "Lange Nacht der Forschung", University of Innsbruck, Austria

Since 2015 "Junge Uni", University of Innsbruck, Austria

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

## Peer-Reviewed Publications

### Under Revision

1. 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*, (2019), submitted. <sup>+</sup>equally contributed.

### Accepted

2. 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*, (2019), accepted.
3. 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*, (2019), accepted. <sup>+</sup>equally contributed.

### Published

4. 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 B12-Cofactors", *Angewandte Chemie International Edition*, **58** (2019), 10756 – 10760. DOI: 10.1002/anie.201904713. IF: 12.1. <sup>+</sup>equally contributed.
5. Katharina Herz, Maren Podewitz<sup>\*</sup>, Laura Stöhr, Dongren Wang, Wolfgang Frey, Klaus R. Liedl, Suman Sen, Michael R. Buchmeiser<sup>\*</sup>. "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. IF: 14.4, Times Cited: 0.  
Corresponding Author: First Corresponding Authorship on a JACS Paper of the Institute of Theoretical Chemistry since 2010.
6. 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: 5.2, Times Cited: 4.
7. 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<sup>-</sup>(H<sub>2</sub>) and Cl<sup>-</sup>(D<sub>2</sub>)", *Journal of Chemical Physics*, **149** (2018), 17310. DOI: 10.1063/1.5049680 IF: 2.8, Times Cited: 1.
8. Maren Podewitz, Yin Wang, 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 IF: 3.2, Times Cited: 1.
9. 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: 3.3, Times Cited: 0.
10. 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: 12.1, Times Cited: 3

11. 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: 5.2 Times Cited: 9.
12. Stefan Vanicek, Maren Podewitz, Christopher Hassenrück, Michael Pittracher, Holger Kopacka, Klaus Wurst, Thomas Müller, Klaus R. Liedl, Rainer F. Winter, Benno Bildstein. "Cobaltocenylidene: A Mesoionic Metallocene Carbene, Stabilized in a Gold (III) Complex", *Chemistry – A European Journal*, **24** (2018), 3165-3169. DOI: 10.1002/chem.201800147. IF: 5.2 Times Cited: 4.
13. 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: 5.2 Times Cited: 0.
14. 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** (2017), 16773-16781. DOI: 10.1002/chem.201704228. IF: 5.2 Times Cited: 7.
15. 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** (2017), 14291-14299. DOI: 10.1021/acs.inorgchem.7b02402. IF: 4.7 Times Cited: 2.
16. 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: 4.1, Times Cited: 5.
17. 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: 2.4 Times Cited: 7.
18. 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: 3.8 Times Cited: 7.
19. 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: 12.1 Times Cited: 11.
20. 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: 5.4 Times Cited: 13.
21. 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: 2.3 Times Cited: 2.
22. 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: 3.4 Times Cited: 23.

23. 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: 1.6 Times Cited: 17.
24. 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: 12.1 Times Cited: 9.
25. 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: 2.4, Times Cited: 3.
26. Carmen Herrmann, Maren Podewitz, Markus Reiher. “Restrained Optimization of Broken-Symmetry Determinants”, *International Journal of Quantum Chemistry*, **109** (2009), 2430–2446. IF: 2.9, Times Cited: 21.
27. 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: 2.2 Times Cited: 40.

### 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. Times Cited: 2.

### 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. Inside Cover:  $\text{Cu}[\text{B}_2(\text{SO}_4)_4]$  and  $\text{Cu}[\text{B}(\text{SO}_4)_2(\text{HSO}_4)]$ —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.
2. 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.
3. Frontispiece:  $\text{CaB}_2\text{S}_4\text{O}_{16}$ : A Borosulfate Exhibiting a New Structure Type with Phyllosilicate Analogue Topology. Jörn Bruns, Maren Podewitz, Michael Schauerperl, Bastian Joachim, Klaus R. Liedl, Hubert Huppertz. DOI: 10.1002/chem.201786664.

4. 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.
5. 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>.
6. 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. "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).
2. "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, 8<sup>th</sup> Carnival Conference Session 2020, February 18 to 20, 2020, Cologne, Germany (**invited**).
2. "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 to August 30, 2019, Cartagena, Colombia (**invited**).

### Past

3. "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 to July 3, 2019, Barcelona, Spain.
4. "Elucidating the Olefin Metathesis Mechanism of A Novel Cationic Molybdenum Catalyst by Quantum Chemistry", March 21, 2019, Federal University of Minas Gerais, Belo Horizonte, Brazil (**invited**).
5. "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**).
6. "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.
7. "Unravelling Reaction Mechanisms with Quantum Chemistry", DK-CIM Winter School, March 4-7, 2018, Obergurgl, Austria (**invited**).
8. "A Novel Mo-Alkylidene Catalyst Facilitates Olefin Metathesis in the Presence of Functional Groups", Polymat 2017, October 15-19, 2017, Huatulco, Mexico (**invited**).
9. "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**).
10. "Novel Mo-Alkylidene Catalysts Can Tolerate Functional Groups in Olefin Metathesis" Gordon Research Seminar: Computational Chemistry, July 2-3, 2016, Girona, Spain.
11. "Solvation and/or Dispersion: The Quest for Accurate Bond Dissociation Energies in B<sub>12</sub> Antivitamins", Boeringer Ingelheim, November 30, 2015, Biberach, Germany.
12. "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.
13. "Spin-Spin Interactions in Biologically Relevant Model Clusters" C4 Workshop IBM, January 19, 2011, Rüslikon, Switzerland.
14. "Understanding Structure and Reactivity of Transition-Metal Clusters", Seminar in Theoretical Chemistry, February 23, 2010, Jerusalem, Israel.
15. "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 STC 2019, 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, Gnadewald, 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.