Prof. Dr Vera Krewald

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Main areas of research

- Theoretical and computational chemistry
- Inorganic & transition metal chemistry
- Theoretical spectroscopy & photochemistry
- Computational catalysis
- Magnetic interactions
- nitrogen (photo)fixation; artificial water oxidation

Education and degrees

08/2014 **Doctorate** in Chemistry, Max Planck Institute for Chemical Energy Conversion, Germany
Supervisors: Prof. Dr Frank Neese and Dr Dimitrios A. Pantazis
Thesis: *Insight into photosynthetic water oxidation through theoretical spectroscopy*

09/2010 **Diploma** (Dipl.-Chem.) in Chemistry, University of Bonn, Germany
Supervisors: Prof. Dr Frank Neese and Dr Dimitrios A. Pantazis
Thesis: *Theoretical magnetochemistry and X-ray absorption spectroscopy of oxo-bridged homo- and heterovalent manganese dimers with multidentate ligands*

06/2005 **Abitur** at Gymnasium Zitadelle der Stadt Jülich, Germany

Employment and academic vita

Since 12/2018 **Professor (W2, tenure track)**
TU Darmstadt, Faculty of Chemistry, Darmstadt, Germany

01/2017–11/2018 **Prize Fellow in the Faculty of Science**
50th Anniversary Prize Fellowship Programme, University of Bath, Dept. of Chemistry, Bath, UK

04/2016–12/2016 **Postdoctoral Researcher**
Research group of Prof. Dr Leticia González
University of Vienna, Faculty of Chemistry, Institute for Theoretical Chemistry, Vienna, Austria

09/2014–03/2016 **Postdoctoral Researcher**
Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany

10/2010–08/2014 **Research Associate**
Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany, & Institute for Physical und Theoretical Chemistry, University of Bonn, Germany

04/2009–09/2010 **Research Assistant**
Institute for Physical und Theoretical Chemistry, University of Bonn, Germany

06/2008–08/2008 **Research Assistant** ('International Research Experience for Undergraduates')
Research group of Prof. Dr Branka M. Ladanyi
Colorado State University, Dept. of Chemistry, Fort Collins, USA

Prizes and awards

2018 Poster award in "Fundamental and applied aspects of N_2 coordination chemistry" at the 43rd International Conference on Coordination Chemistry (ICCC) in Sendai, Japan

2015 Otto Hahn Medal 2014 for '*New insights into the structural basis of water oxidation in photosynthesis*'

2014	Poster award at the conference 'Interfaces between experimental and theoretical approaches to energy-related enzyme catalysis', London, UK
2013	Participation in the 63rd Lindau Nobel Laureate Meeting, funded by the Max Planck Society
2008 – 2013	Scholarships from Studienstiftung des Deutschen Volkes (German National Academic Foundation) at undergraduate and PhD level

Funding received

2016	Marie-Skłodowska-Curie Individual Fellowship for 24 months under the European Union (EU) Horizon 2020 call H2020-MSCA-IF-2015 Project 'Solar Dinitrogen Activation' (acronym SolarAct, grant agreement no. 703860), together with Prof. Dr Leticia González, University of Vienna, and in collaboration with Prof. Dr Markus Reiher, ETH Zürich
2008	Scholarship from German Academic Exchange Service (DAAD, Germany) and National Science Foundation (NSF, USA) to participate in the International Research Experience for Undergraduates program; carried out research with Prof. Dr Branka M. Ladanyi, Colorado State University, USA

Services to the scientific community

09/2018	Host of the *4th Quantum Bio•Inorganic Chemistry Conference* (QBIC•IV)
2017– today	Reviewer for scientific journals and international scientific funders

Activities in professional societies

04/2018– today	Co-founder and Secretary General of the *Quantum Bio-Inorganic Chemistry Society e.V.* (http://qbicsoc.org)
07/2016– 10/2018	Gesellschaft Deutscher Chemiker (Ordentliches Jungmitglied)
12/2016– today	Royal Society of Chemistry (MRSC)

Darmstadt, 31.01.2018

List of Invited and Contributed Presentations

- *TBA*
  17th Central European Symposium on Theoretical Chemistry in Burg Schlaining, Austria, ***09/2019*** (invited)
- *TBA*
  CECAM workshop "Theoretical and Computational Inorganic Photochemistry: Methodological Developments, Applications and Interplay with Experiments" in Toulouse, France, ***06/2019*** (invited)
- *TBA*
  CanBIC-7 in Parry Sound, Canada, ***05/2019*** (invited)

17. "Theoretical Insights into Nitrogen Photoactivation"
    Departmental seminar at Göttingen University, ***12/2018*** (invited)
16. "*On the Nature of the Active Species in O-O Bond Formation in Natural Water Oxidation*"
    Oral speaker at 43rd International Conference on Coordination Chemistry (ICCC), ***08/2018***
15. "*Progress in understanding dinitrogen photocleavage*"
    Departmental seminar at Queen-Mary University London, ***02/2018*** (invited)
14. "*Progress in understanding dinitrogen photocleavage*"
    ECOSTBio (Explicit Control over Spin-states in Technology and Biochemistry) seventh scientific meeting in Dublin, Ireland, ***12/2017***
13. "*Electronic structure analysis of transition metal dimers for dinitrogen photocleavage*" (invited)
    Ruhr-Universität Bochum, Germany, ***11/2017***
12. "*Electronic structure analysis of transition metal dimers for dinitrogen photocleavage*"
    ISACS: Challenges in Inorganic Chemistry in Manchester, UK, ***04/2017***
11. "*Electronic structure investigation of osmium and molybdenum dimers capable of dinitrogen photocleavage*"
    25. Lecture Conference on Photochemistry in Jena, Germany, ***09/2016***
10. "*Electronic structure analysis of transition metal dimers for dinitrogen photocleavage*"
    ECOSTBio (Explicit Control over Spin-states in Technology and Biochemistry) fifth scientific meeting in Kraków, Poland, ***09/2016***
09. "*In silico design of catalytic entities: electronic structure analysis of dinitrogen photocleavage catalysts and redox accumulating manganese complexes*"
    MICRA (Meeting of Inorganic Chemists Recently Appointed) in Bath, UK, ***09/2016***
08. "*Prediction of redox potentials for magnetically coupled transition metal clusters*"
    51st Symposium on Theoretical Chemistry in Potsdam, Germany, ***09/2015***
07. "*Spectroscopically consistent Mn oxidation state assignments of the natural water splitting catalyst*"
    Group seminar of Prof. Dr. L. González in Vienna, Austria, ***03/2015*** (invited)
06. "*Magnetic interactions in nature's water splitting complex and synthetic analogues*"
    ECOSTBio (Explicit Control over Spin-states in Technology and Biochemistry) first scientific meeting in Girona, Spain, ***09/2014***
05. "*Spectroscopically consistent Mn oxidation state assignments of the natural water splitting catalyst*"
    12th European Biological Inorganic Chemistry Conference in Zürich, Switzerland, ***09/2014***
04. "*Spectroscopically consistent Mn oxidation state assignments of the natural water splitting catalyst*", including an educational introduction to magnetic interactions in transition metal complexes and their calculation with broken symmetry DFT
    3rd Bioinorganic Training Workshop at Pennsylvania State University, University Park, USA, ***06/2014***

03. "*Magnetic properties of high-valent Mn_3CaO_4 cubane complexes*"
    Jujols VII in Mülheim an der Ruhr, Germany, ***01/2014***
02. "*X-ray absorption and emission spectroscopy on models of the oxygen evolving complex and related compounds*"
    2nd Bioinorganic Training Workshop at Penn State University, University Park, USA, ***06/2012***
01. "*Theoretical magnetochemistry and X-ray absorption spectroscopy of manganese dimers*"
    Jujols V in Tarragona, Spain, ***11/2010***

Poster presentations

08/2018: 43rd International Conference on Coordination Chemistry (ICCC)

08/2016: 17th Intl. Congress on Photosynthesis Research, Maastricht, NL

04/2015: 1st Intl. Solar Fuels Conference, Uppsala, SE;

03/2015: Computational Molecular Science, Warwick, GB

06/2014: Interfaces between experimental and theoretical approaches to energy-related enzyme catalysis, London, GB

06/2014: 3rd Bioinorganic Training Workshop, Penn State University, US

07/2013: International Conference on Bioinorganic Chemistry 16, Grenoble, FR

06/2013: Ab Initio Molecular Dynamics for Biomolecules summer school, l'Aquila, IT

01/2013: 6th Advanced EPR School of EFEPR, Weizmann Institute of Science, Rehovot, IL

09/2012: 48th Symposium on Theoretical Chemistry, Karlsruhe, DE

07/2011: 9th Triennial Congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostela, ES

06/2011: Quantum Bioinorganic Chemistry 3, Cesky Krumlov, CZ

03/2011: Modeling Natural and Artificial Photosynthesis, Leiden, NL

09/2010: 46th Symposium on Theoretical Chemistry, Münster, DE