

Prof. Dr. Vera Krewald

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Date and place of birth: May 1987 in Aachen, Germany

Research profile

- ◆ Theoretical and Quantum Chemistry
- ◆ Magnetic interactions and theoretical spectroscopy
- ◆ Computational catalysis, photochemistry and electron transfer

Employment and academic vita

Since 11/2023	Professor for Quantum Chemistry (W3) TU Darmstadt, Dept. of Chemistry
12/2018–10/2023	Professor for Theoretical Chemistry (W2, tenure track 12/2018–11/2022) TU Darmstadt, Dept. of Chemistry
01/2017–11/2018	Research Group Leader in the Faculty of Science (50 th Anniversary Prize Fellowship) University of Bath, Dept. of Chemistry
04/2016–12/2016	Postdoctoral Researcher (Marie-S.-Curie fellowship) Prof. Dr. Dr. h.c. L. González, University of Vienna, Faculty of Chemistry
09/2014–03/2016	Postdoctoral Researcher Prof. Dr. F. Neese, Dr. D. A. Pantazis, MPI CEC, Mülheim/Ruhr
10/2010–08/2014	Research Assistant (PhD student) Prof. Dr. F. Neese, Dr. D. A. Pantazis, MPI CEC, Mülheim/Ruhr; IPTC, University of Bonn

Education and degrees

08/2014	Doctorate (Dr. rer. nat.) in Chemistry Prof. Dr. F. Neese, Dr. D. A. Pantazis, MPI CEC, Mülheim/Ruhr and University of Bonn
09/2010	Diploma (Dipl.-Chem.) in Chemistry Prof. Dr. F. Neese, Dr. D. A. Pantazis, University of Bonn

Prizes and awards

2022	Dozentenpreis, award of the chemical industry fund within the German chemical industry association (Fonds der Chemischen Industrie, VCI)
2021	Award of the Dr. Hans Messer Stiftung for early career researchers at TU Darmstadt
2021	ADUC Award of the German association of university professors in chemistry in the Gesellschaft Deutscher Chemiker (GDCh)
2014	Otto Hahn Medal of the Max-Planck-Society
2013	Participant at 63 rd Lindau Nobel Laureate Meeting
2008–2013	German National Academic Foundation (Studienstiftung des Deutschen Volkes)

Key research data

- ◆ Leader of a research group with 2 postdocs, 6 PhD candidates, several B.Sc./M.Sc. students
- ◆ 59 peer-reviewed research articles, reviews and book chapters, 32 as corresponding author
- ◆ Funding from DFG, Leverhulme Trust, Merck'sche Gesellschaft für Kunst und Wissenschaft e.V., NHR Verein e.V., Deutsche Bundesstiftung Umwelt
- ◆ Vice-speaker of SFB 1487 „Iron, upgraded!“ (2022–2025); speaker U. I. Kramm, vice-speaker C. Hess

Invited conference and seminar presentations (selection)

- (09/2024) 7th European Colloquium on Inorganic Reaction Mechanisms, Toulouse, France
- 08/2024 17th European Biological Inorganic Chemistry Conference EuroBIC-17, Münster, Germany
- 05/2024 13th ESPA (Electronic Structure: Principles and Applications), Tarragona, Spain
- 09/2023 5th Conference of Theory and Applications of Computational Chemistry (TACC), Japan
- 08/2023 Quantum Bio-Inorganic Chemistry VI, Warsaw, Poland
- 07/2022 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Canada
- 05/2022 Computational Catalysis Lecture Series, IIT Roorkee, India (virtual lecture)
- 09/2021 CataLight Young Scientist Symposium (TRR234)

Lecturing and teaching (selection)

- Since 2019 *Quantum Chemistry I, Quantum Chemistry II, Quantum Mechanics and Symmetry* (M.Sc.)
Computational Applications in Chemistry (B.Sc., 50%)
- 2018 Fellow of the Higher Education Academy, UK Professional Standards Framework
- 2017–2018 *Introduction to Computational Chemistry*, University of Bath, 2nd Year, 50%
Computational Chemistry Laboratories, University of Bath, 2nd/4th Year, 25%

Academic self-governance and commissions of trust (selection)

- Since 2024 Member of the Hellmann committee for early career researcher awards of AG Theoretische Chemie (AGTC; main organisation for theoretical chemistry in German-speaking countries)
- Since 2024 Member of the selection committee on early career researcher awards at TU Darmstadt
- Since 2023 Elected member of the department council, Dept. of Chemistry, TU Darmstadt
- Since 2022 Elected member, Steering Committee of the research field *Matter&Materials* at TUDa
- Since 2022 Member of the departmental committee on quality assurance funds for teaching
- Since 2021 Representative in the *Unite!* Academic Forum
- Since 2021 Member of the NHR₄CES Resource Allocation Board
- 2022–2024 Member of ESRF Beamtime Allocation Panel C11

Services to the scientific community

- Since 2024 *JACS Au* Early Career Advisory Board
- 2022/2023 Guest editor special issue "Inorganic Reaction Mechanisms" of *Eur. J. Inorg. Chem.* (Wiley)
- 2020/21/22 Co-organiser Lorentz Center workshop „Quantum Bio-Inorganic Chemistry“
- 2019/2020 Guest editor special issue "Germany's Future in Theoretical and Computational Chemistry: a Special Issue Celebrating DEAL" of the *International Journal of Quantum Chemistry* (Wiley)
- Since 2018 Co-founder, Secretary General of *Quantum Bio-Inorganic Chemistry Society e.V.*; qbicsoc.org
- 09/2018 Host of the Quantum Bio-Inorganic Chemistry IV Conference (QBIC-IV)
- Since 2017 Reviewer for scientific journals and international scientific funders (incl. DFG, US DoE, NCN)



Darmstadt, September 2024