

Prof. Dr. Frank Neese

<https://www.kofo.mpg.de/de/forschung/molekulare-theorie-und-spektroskopie>

Short Biography

Frank Neese received both his Diploma (Biology – 1993) and PH.D (Dr. rer. Nat. – 1997) working with Prof. P. Kroneck at the University of Konstanz. He performed Postdoctoral work at Stanford University with Prof. E. I. Solomon from 1997 to 1999, then returned to Konstanz where he completed his Habilitation in 2001. He joined the Max Planck Institute (MPI) for Bioinorganic Chemistry in 2001 as a group leader, where he directed a research group until accepting the position of Chair of Theoretical Chemistry at the University of Bonn in 2006. In 2008, Neese returned part time to the MPI as one of its rare “Max Planck Fellows” within the Department of Inorganic Chemistry. In 2011, he became Director of the MPI for Chemical Energy Conversion where he was leading an interdisciplinary group that combines spectroscopy and theory in development and application. In 2018, Neese was appointed Director of the Max Planck Institute of Coal Research where he heads the department of Molecular Theory and Spectroscopy as the successor of the late Professor Walter Thiel. He holds honorary professorships at the University of Bonn and Duisburg-Essen. In 2005, Prof. Neese received the Hellmann Award of the German Theoretical Chemical Society for the Development and Application of new Theoretical Methods and subsequently the Klung-Wilhelmy Weberbank award in 2008 and the Gottfried Wilhelm Leibniz Award of the German Science foundation in 2010. Neese is member of various national and international academies including the Northrhine Westfalia Academy of Science (2020), the German National Academy of Sciences (Leopoldina, 2013), The Academia Europaea (2018) and the International Academy of Quantum Molecular Science (2012). Neese was Associate Editor (2011-2014) of the journal *PhysChemChemPhys*, since 2015, of the journal *Inorg. Chem.*. Frank Neese served on numerous scientific committees including the Central Review panel of the German Science Foundation, the Kuratorium of the German “Fonds der Chemie”, the Advisory Board for the Institute of Organic Chemistry and Biochemistry (IOCB) of the Czech Academy of Sciences in Prague and the Fritz-Haber Center in Jerusalem. Neese is the author of more than 580 scientific articles in journals of Chemistry, Biochemistry and Physics. His work focuses on the theory of magnetic spectroscopies (electron paramagnetic resonance, magnetic circular dichroism) and their experimental and theoretical application, local pair natural orbital correlation theories, spectroscopy oriented configuration interaction, electronic and geometric structure and reactivity of transition metal complexes and metalloenzymes. He is the designer and lead author of the ORCA program, which is presently the second most widely used quantum chemistry package worldwide.