Leopoldina
Nationale Akademie
der Wissenschaften

Curriculum Vitae Professor Dr. Walter Thiel

Name: **Walter Thiel**
Born: **7 March 1949** **Deceased: 23 August 2019**

Academic and Professional Career

since 2001	Honorary Professor, University Düsseldorf, Germany
since 1999	Director, Max Planck Institute for Coal Research, Germany
1992 - 1999	Full Professor, University Zurich, Switzerland
1987	Visiting Professor, University of California at Berkeley, USA
1983 - 1992	Associate Professor, University Wuppertal, Germany
1981	Habilitation, University Marburg, Germany
1973 - 1975	Postdoctoral fellow, University of Texas at Austin (M.J.S. Dewar), USA
1971 - 1973	Doctoral studies, University Marburg (A. Schweig), Germany
1966 - 1971	Chemistry studies, University Marburg, Germany

Project coordination, Membership in collaborative research projects (Selection)

2006 - 2010	MPG project, Triple-M: Multiscale Materials Modeling
2005 - 2013	Volkswagenstiftung: QM / MM Methods for Biomolecular Simulation
2005 - 2010	DFG project, SFB 663: Electronically Excited States in Large Molecules
2005 - 2009	EU project: Quantitative Spectroscopy for Atmospheric and Astrophysical Research
2004 - 2008	Coordinator, DIP project: Asymmetric Catalysis
2000 - 2003	EU project: Spectroscopy of Highly Excited Rovibrational States

1998 - 2001 EU project: Quantum Simulations in Industry

Functions in Scientific Societies and Committees (Selection)

since 2012 Member of the Board of Governors, German Chemical Society

since 2012 Editorial Advisory Board, Accounts of Chemical Research

since 2012 Editorial Advisory Board, ACS Catalysis

since 2011 President, World Association of Theoretical and Computational Chemists

2010 Chairman, Gordon Conference on Computational Chemistry

since 2009 Member of the International Advisory Board, State Key Laboratory of Physical Chemistry (PCOSS), Xiamen, China

since 2008 Associate Editor, WIRES: Computational Molecular Sciences

since 2006 Member of the Curatorium, Chemistry

2006 - 2012 Chairman, BAR Committee of the Max Planck Society

2006 - 2008 Managing Director, Max Planck Institute for Coal Research

since 2004 Member of the Scientific Advisory Board, Lise Meitner Minerva Center for Quantum Chemistry, Jerusalem, Haifa, Israel

2004 - 2007 Member, Standing Commitee of the Bunsen Society

2002 - 2008 Section Editor, Encyclopedia of Computational Chemistry

2001 - 2005 Chairman, Working Group for Theoretical Chemistry

2000 - 2006 Member of the Steering Committee, Bavarian Supercomputer Center

2000 - 2008 Member of the Review Board, German Research Foundation

since 1998 Advisory Editor, Journal of Computational Chemistry

since 1997 Advisory Editor, Theoretical Chemistry Accounts

1986 - 1992 Member of the Board, Institute for Informatics, Wuppertal, Germany

Honours and Awarded Memberships (Selection)

2012 Liebig Medal, German Chemical Society

2008 Member, North Rhine-Westphalia Academy for Sciences and Arts

2007 Member, International Academy of Quantum Molecular Sciences

2007 Member, German Academy of Sciences Leopoldina

2002	Schrödinger Medal, World Association of Theoretical Chemists
1988	Promoting Award, Alfried Krupp Foundation
1982	Heisenberg Fellowship, German Research Foundation
1975	Liebig Fellowship, Association of the Chemical Industries

Major Scientific Interests

Our central field of research is Theoretical Chemistry, in particular Quantum Chemistry. We focus on theoretical developments that extend the scope of computational methodology, especially for large molecules, and we apply theoretical methods to study specific chemical problems, mostly in close cooperation with experimental partners. Our activities cover a broad methodological spectrum, including ab initio methods, density functional theory, semiempirical methods, and combined quantum mechanical/molecular mechanical approaches.

Recent applications from these areas address the rovibrational spectra of small molecules, catalytic reactions of transition metal compounds, excited-state dynamics, and enzymatic reactions. They thus range from accurate calculations on small molecules to the approximate modeling of very complex systems with thousands of atoms.